An alternative to the conventional micro-canonical ensemble

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Abstract

The usual approach to the foundations of quantum statistical physics is based on the conventional micro-canonical ensemble as a starting point for deriving the Boltzmann–Gibbs (BG) equilibrium. It leaves, however, a number of conceptual and practical questions unanswered. Here we discuss these questions, thereby motivating the study of a natural alternative known as the quantum micro-canonical (QMC) ensemble. We present a detailed numerical study of the properties of the QMC ensemble for finite quantum systems, revealing good agreement with the existing analytical results for large quantum systems. We also propose the way to introduce analytical corrections accounting for finite-size effects. With the above corrections, the agreement between the analytical and the numerical results becomes very accurate. We demonstrate that the variance of energy fluctuations can be used to discriminate the QMC equilibrium from the BG equilibrium.

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((Some figures may appear in color only in the online journal)

1. Introduction

This paper is about a quantum statistical ensemble, which is, in a sense, opposite to the conventional micro-canonical ensemble. It is an extension of the previous work of one of us [1]. The present work contains a discussion of the underlying conceptual issues and detailed analytical and numerical investigations on finite quantum systems.

The standard quantum-mechanical derivation of the Boltzmann–Gibbs (BG) equilibrium is based on the conventional micro-canonical postulate formulated as follows. One should consider a subsystem in a macroscopic environment, assume that the two form an isolated macroscopic system, neglect the interaction between them and then select the statistical ensemble amounting to an incoherent mixture of eigenstates of the total system in a narrow energy window around a given value of energy, \(E_{\text{av}}\). The width of this micro-canonical energy window \(\Delta_{\text{mc}}\) should be large enough to include a very large number of quantum levels, but, at the same time, small enough to imply a negligible change in temperature across this energy window. With the above micro-canonical ensemble, the temperature \(T\) of a small subsystem as a function of \(E_{\text{av}}\)
can be determined as

\[
\frac{1}{T(E_{\text{av}})} = \frac{\partial \log[\nu(E)/\nu_0]}{\partial E} \bigg|_{E=E_{\text{av}}},
\]

where \(\nu(E)\) is the density of energy states of the system and \(\nu_0\) is an unimportant normalization constant.

Recently, further progress was made by showing that a single pure state of a macroscopic system formed by a coherent superposition of eigenstates randomly selected from the above energy window would also lead to a density matrix of the subsystem exhibiting the BG distribution [2–5]. It has been further conjectured that if the isolated macroscopic system is chaotic in the classical limit, then even a single eigenstate would lead to the BG distribution in the density matrix of the subsystem [6].

However, the question remains: what is the justification for the narrow energy window in the micro-canonical postulate? It could have been that the narrow energy condition is only a simplification, while the BG distribution emerges for a broader class of ensembles. One can, in particular, recall that the conventional canonical ensemble does not appear to have a narrow energy window for participating eigenstates.
To each eigenstate with energy $E$, it assigns probability weight $p(E) \equiv \exp(-E/T_0)$, where $T_0$ is a constant. Here, it should be noted, however, that the quantity of practical interest is not the probability weight function $p(E)$ as such but rather its product with the density of states $\nu(E)$. Since $p(E)$ decays exponentially with constant ‘rate’ $1/T_0$, while for a macroscopic system $\nu(E)$ increases exponentially with decreasing ‘rate’ $1/T(E)$, the product $p(E)\nu(E)$ would have a narrow maximum at energy $E = E_\text{av}$ corresponding to $T(T_0) = T_0$. The width of that maximum $\Delta_c$ is determined by the second derivative of $\log \nu(E)$

$$\left. \frac{\partial^2 \log \nu(E)/\nu_0}{\partial E^2} \right|_{E = E_\text{av}} \sim -\frac{1}{T_0^2 N_p},$$

where $N_p$ is the number of particles in the system. This gives $\Delta_c \sim T_0/\sqrt{N_p}$. As a result,

$$-\Delta_c \left. \frac{\partial [1/T(E)]}{\partial E} \right|_{E = E_\text{av}} \sim -\frac{1}{T_0^2 \sqrt{N_p}} \ll \frac{1}{T_0},$$

i.e. the temperature does not strongly vary when the energy changes by $\Delta_c$. Thus the canonical ensemble implicitly imposes a narrow energy window on the function $p(E)\nu(E)$.

As discussed in [1, 7], the departure from the above narrow energy condition easily spoils the BG statistics for a subsystem. It leads to a mixture of different thermal distributions, which does not produce a distribution characterized by a single temperature. The basic concern in the context of the foundations of statistical physics remains about the actual behavior of an isolated quantum system perturbed from equilibrium and not interacting with a large thermal bath. If, after the perturbation, an isolated quantum system is in a broad superposition of eigenstates violating the narrow energy condition, then the occupation numbers of eigenstates will not change with time under the dynamics guided by the linear Schrödinger equation and hence the narrow energy condition will never emerge.

To address the issue of what might happen without the narrow energy constraint, an ensemble with the unrestricted participation of eigenstates, referred to below as the quantum micro-canonical (QMC) ensemble [1, 8–10], is a conceptually necessary limit to consider. (Similar quantum canonical ensembles have also been defined in [8, 11].) This ensemble is also important because it was shown to be realizable in small isolated quantum systems with a large number of quantum levels [12]. Beyond the subject of the foundations of quantum statistical physics, the properties of the QMC ensemble are relevant to the studies of various properties of the Hilbert spaces, e.g. in the context of quantum computing or many-particle entanglement. It is finally plausible, on general grounds, that such a natural quantum ensemble would find many realizations not discovered so far. For example, it has been demonstrated in [1] that the expansion of the basis states of sparse random matrices in terms of eigenstates exhibits QMC-type statistics.

In section 2, we summarize the analytical results obtained in [1] for the QMC ensemble in large-$N$ quantum systems. In section 3, we propose a method of introducing finite-$N$ corrections to the results of [1]. In section 4, we present numerical tests of the above method for a 12-level quantum system. In section 5, we examine numerically the density matrix for a subsystem of a 12-level system, and compare the QMC-based result with that of the conventional canonical ensemble.

2. Quantum micro canonical (QMC) ensemble

We consider a quantum system having a large but finite number $N$ of energy levels. The eigenenergies $\{E_i\}$ of this system are ordered according to their values. We define $E_{\text{min}} \equiv E_1$ and $E_{\text{max}} \equiv E_N$. The generic wave function $\Psi$ of such a system is a superposition of eigenstates $\phi_i$:

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

where $C_i$ are complex amplitudes. For an isolated quantum system, fixing the energy expectation value $E_{\text{av}}$ associated with the wave function $\Psi$ implies

$$\sum_{i=1}^N E_i |p_i = E_{\text{av}},$$

where $p_i = |C_i|^2$ are the occupation numbers of quantum eigenstates. We shall denote by $E_{\text{av}}$ the ‘average energy’ (not to be confused with the uniform average of all $E_i$).

The QMC ensemble includes all possible quantum wave functions satisfying the average energy constraint (4). Formally, it is defined by specifying a uniform joint probability distribution for complex amplitudes $C_i \equiv |C_i| e^{\phi_i}$ in the Hilbert space—subject to average energy constraint (4) and to the normalization constraint

$$\sum_{i=1}^N p_i = 1.$$
Since constraints (4) and (5) do not depend on \( \varphi_i \), the assignment of variables \( \varphi_i \) is totally random. The resulting uniform distribution of \( \varphi_i \) can be just factorized out and then integrated. What remains is the Euclidean subspace of variables \( p_i \) with uniform joint probability measure on the manifold constrained by conditions (4) and (5) together with the positivity condition

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

In the \( p_i \)-space, due to the linear nature of constraints (4), (5) and (7), the boundaries of the resulting manifold are flat, i.e. the manifold itself is an \( (N - 2) \)-dimensional polyhedron.

We will denote it as the ‘QMC polyhedron’. Our goal is to obtain the marginal probability distribution \( P_k(p_k) \) for a given occupation number \( p_k \) and the corresponding average value \( \langle p_k \rangle \) representing the participation of the \( k \)-th eigenstate in the QMC ensemble.

The probability distribution \( P_k(p_k) \) is proportional to the \((N - 3)\)-dimensional volume of the intersection of the QMC polyhedron with the hyperplane \( p_k = \text{const} \).

Here we use variable \( p_k \) as a label of the coordinate axis, while in \( P_k(p_k) \) and everywhere below, \( p_k \) denotes the value of const.

The intersection manifold is to be denoted as \( M_k \), and its volume as \( V_k(p_k) \). This volume plays the role of unnormalized probability distribution such that

\[ P_k(p_k) = \frac{V_k(p_k)}{\int_0^1 V_k(p'_k)\,dp'_k}, \tag{8} \]

and the average value of \( p_k \) is

\[ \langle p_k \rangle = \frac{\int_0^1 p'_k V_k(p'_k)\,dp'_k}{\int_0^1 V_k(p'_k)\,dp'_k}. \tag{9} \]

The most relevant limit to consider now is \( p_k \ll 1 \), because, for \( N \gg 1 \), it is improbable that a single occupation number \( p_k \) in a randomly chosen superposition of all quantum states becomes comparable to 1. We denote this limit as ‘small-\( p_k \) approximation’. It gives [1]

\[ V_k(p_k) = V_k(0) e^{-N p_k[1+\lambda_k(E_k-E_{av})]}, \tag{10} \]

where \( \lambda_k \) is the volume renormalization parameter associated with the shift of the energy hyperplane (4). The corresponding average occupation number is

\[ \langle p_k \rangle = \frac{1}{N[1+\lambda_k(E_k-E_{av})]} . \tag{11} \]

The value of the parameter \( \lambda \) can now be found numerically by substituting equation (11) into the average energy condition

\[ \sum_{k=1}^N (E_k - E_{av}) \langle p_k \rangle = 0. \tag{12} \]

Equation (10) can be viewed as describing a grand canonical ensemble in the Hilbert space with the chemical potential

\[ E_\lambda = E_{av} - \frac{1}{\lambda} \tag{13} \]

and the inverse temperature \( \lambda N \).

The value of \( \lambda \) is zero when \( E_\lambda \) is equal to \( E_{av0} \), the uniform average of all energies in spectrum \( \{ E_i \} \) [1, 10]:

\[ E_{av0} = \frac{1}{N} \sum_{i=1}^N E_i. \tag{14} \]

We also recall that \( \lambda > 0 \) for \( E_{av} < E_{av0} \), and \( \lambda < 0 \) for \( E_{av} > E_{av0} \). Below, unless specified otherwise, the origin of the energy axis is set at \( E_{av0} \).

The chemical potential \( E_\lambda \) is simultaneously the pole of the function \( \langle p_k \rangle(E_{av}) \) given by equation (11), which implies that for the small-\( p_k \) approximation to be valid for all levels, \( E_\lambda \) should be sufficiently below the lowest energy level for positive \( \lambda \) or above the highest energy level for negative \( \lambda \). In the former case, ‘sufficiently below’ means that [1]

\[ E_{min} - E_\lambda \gg \frac{E_{av} - E_{min}}{N}. \tag{15} \]

It is shown in [1] that the above condition is violated for a typical macroscopic system at a typical value of \( E_{av} \), which leads to condensation into the lowest energy state, i.e. \( \langle p_i \rangle \) becomes comparable to 1. Condition (15) can also be easily violated for finite-\( N \) systems leading to the departure from the small-\( p_k \) results (10) and (11) for several lowest levels.

When the typical values of \( p_k \) are not small, the parameters \( \lambda_k \) are defined as functions of the average energy \( E_{av} \) as follows [1]:

\[ \lambda_k[E_{av}] = \frac{1}{V_k} \frac{\partial V_k}{\partial v}_{|v=0}, \tag{16} \]

where (in this equation alone) \( V_k \) is the volume of the manifold constrained in the space of all variables excluding \( p_k \)—to be denoted as \( [p_i]_k \)—by the conditions

\[ \sum_{i,i\neq k}^N p_i = 1, \tag{17} \]

\[ \sum_{i,i\neq k}^N (E_i - E_{av}) p_i = v, \tag{18} \]

together with positivity conditions (7). Here \( v \) is the energy shift parameter. We use square brackets to enclose arguments in functions \( \lambda_k[E_{av}] \) and later in \( \lambda[E_{av}] \).

Given the above definition of \( \lambda_k[E_{av}] \), the volume of manifold \( M_k \) defined by equations (7), (17) and (18) can be expressed as

\[ V_k(p_k) = V_k(0) \exp \left[ (N-3) \log(1-p_k) + \int_{E_{av}}^{E_{av}-(E_k-E_{av})/p_k} \lambda_k[E] \,dE \right]. \tag{19} \]

(This equation does not appear explicitly in [1], but otherwise it is an obvious intermediate step in the calculation described there.) In the limit \( N \gg 1 \), all \( \lambda_k[E] \) are approximately equal to a single function \( \lambda[E] \) defined in the interval \([E_{min}, E_{max}]\).
Therefore, equation (19) becomes [1]

\[ V_k(p_k) = V_k(0) \exp \left\{ (N-3) \left[ \log(1-p_k) + \int_{E_{av}}^{\infty} \frac{\lambda(E) dE}{(E_k-E_{av})p_k} \right] \right\}. \]

Functions \( V_k(p_k) \) given by both equations (19) and (20) are not necessarily defined in the entire range \( 0 \leq p_k \leq 1 \), because, for too large \( p_k \), and, in the case of \( k = 1 \) or \( k = N \), for too small \( p_k \), the intersection manifold \( \mathcal{M}_k \) may simply not exist. The practical rule is that \( V_k(p_k) \) is defined, when \( \lambda_k[E] \) or \( \lambda(E) \) are defined at the upper integration limit \( E_{av} = \frac{(E_k-E_{av})p_k}{1-p_k} \). This limit should fall within interval \([E_{min}, E_{max}]\) for equation (20) and within sometimes different boundaries (given in section 3) for equation (19). The upper cutoffs for \( p_k \) are given in appendix D of [1] and the lower cutoffs in section 3. The mean-\( \lambda \) approximation represented by equation (20) neglects the existence of lower cutoffs of \( p_k \) for \( k = 1 \) and \( k = N \). These cutoffs, however, can be incorporated at the level of finite-\( N \) corrections based on equation (19). If a lower cutoff is present, then \( V_k(0) \) is not defined, and the prefactor in equation (19) should be viewed simply as a constant, which is then canceled by normalization in equation (8). Also, when a lower cutoff is present, the lower integration limit \( E_{av} \) in equation (19) should be replaced with the minimum value or maximum value of energy, where \( \lambda_k[E] \) is defined, for \( k = 1 \) and \( k = N \), respectively. In general, function \( V_k(p_k) \) becomes exponentially small as it approaches either of its cutoffs. Therefore, as \( N \) increases, the practical significance of these cutoffs decreases.

In equation (20), we took, at first sight inconsistently, the large-\( N \) limit \( \lambda_k[E] \approx \lambda(E) \) but did not approximate \( N - 3 \approx N \). The reason is that we are aiming at making numerical tests for the Hilbert space with \( N \sim 10 \), where condition \( N - 3 \gg 1 \) is not well fulfilled, and since the term \((N-3) \log(1-p_k)\) is an exact one [1], we thereby limit the finite-\( N \) error only to the integral in equation (20) and deal with this error later in section 3.

Equation (20) was the basis for proving the condensation of the QMC ensemble into the lowest energy state of macroscopic systems [1]. It indicated that the character of function \( V_k(p_k) \) was not exponential but rather narrowly peaked around \( p_k = \langle p_k \rangle \).

### 3. Deviations of \( \lambda_k[E_{av}] \) from \( \lambda[E_{av}] \)

While we cannot propose a controllable procedure for finding corrections for \( \lambda_k[E_{av}] \) with respect to \( \lambda[E_{av}] \), we introduce here an ansatz, which makes these corrections in a meaningful way and, at the same time, significantly improves the agreement with Monte-Carlo results.

The ansatz is based on the following considerations. Function \( \lambda[E_{av}] \) is defined in interval \([E_{min}, E_{max}]\). It has two universal properties in the large-\( N \) limit [1]:

1. \( \lambda[E_{av}] = 0 \);
2. for \( E_{av} < E_{av0} \), \( \lambda[E_{av}] \) quickly approaches the asymptotic form

\[ \lambda[E_{av}] \approx \frac{1}{E_{av} - E_{min}}, \]

while for \( E_{av} > E_{av0} \), the asymptotic form is

\[ \lambda[E_{av}] \approx \frac{1}{E_{av} - E_{max}}. \]

In other words, the behavior of the entire function \( \lambda[E_{av}] \) is almost entirely determined just by the values of three parameters \( E_{av0}, E_{min} \) and \( E_{max} \).

Now, function \( \lambda_k[E_{av}] \) characterizes the entire quantum spectrum \( \{E_k\} \), while functions \( \lambda_k[E_{av}] \) characterize spectra \( \{E_k\} \) obtained from \( \{E_k\} \) by removing the energy level \( E_k \). As a result, the uniform average of all energies for spectrum \( \{E_k\} \) is shifted to

\[ E_{av0k} = E_{av0} + \frac{E_{av0} - E_k}{N-1}, \]

while the end points of the spectrum remain unchanged, unless \( k = 1 \) or \( k = N \), when, respectively, the minimum or the maximum energy levels are removed:

\[ E_{mink} = \begin{cases} E_2 & k = 1, \\ E_{min} & k > 1, \end{cases} \]

\[ E_{maxk} = \begin{cases} E_{max} & k < N, \\ E_{N-1} & k = N. \end{cases} \]

Apart from the above specific differences, \( \lambda_k[E_{av}] \) should be reminiscent of \( \lambda[E_{av}] \). Therefore, in order to approximate \( \lambda_k[E_{av}] \) from the knowledge of \( \lambda[E_{av}] \) we adopt the following two-step procedure:

(I) Shift of \( \lambda[E_{av}] \) to move \( E_{av} \) to \( E_{av0k} \):

\[ \lambda_k'[E_{av}] = \lambda[E_{av0} + E_{av0} - E_{av0k}]. \]

This also shifts \( E_{min} \) and \( E_{max} \) (the end points of \( \lambda[E_{av}] \)) to \( E_{mink} = E_{min} + E_{av0} - E_{av0k} \) and \( E_{maxk} = E_{max} + E_{av0} - E_{av0k} \), respectively.

(II) Uniform contraction or expansion of energy differences above and below \( E_{av0k} \) to shift \( E_{mink} \) and \( E_{maxk} \) to, respectively, \( E_{min} \) and \( E_{max} \) given by equations (23) and (24) and simultaneously rescale \( \lambda_k' \) itself to make sure that if \( \lambda_k'[E_{av}] \) has asymptotic forms \( \frac{1}{E_{av} - E_{min}} \) above \( E_{mink} \) and \( \frac{1}{E_{av} - E_{maxk}} \) below \( E_{maxk} \), then the resulting function \( \lambda_k[E_{av}] \) has the asymptotic forms \( \frac{1}{E_{av} - E_{min}} \) above \( E_{mink} \) and \( \frac{1}{E_{av} - E_{maxk}} \) below \( E_{maxk} \). This transformation is

\[ \lambda_k[E_{av}] = \begin{cases} \frac{1}{E_{av} - E_{av0k} + \alpha_-(E_{av0} - E_{av0k})} & E_{av} < E_{av0}, \\ \frac{1}{E_{av} - E_{av0k} + \alpha_+(E_{av} - E_{av0k})} & E_{av} > E_{av0}, \end{cases} \]

where

\[ \alpha_- = \frac{E_{min} - E_{av0}}{E_{min} - E_{av0k}} \]

\[ \alpha_+ = \frac{E_{max} - E_{av0}}{E_{max} - E_{av0k}}. \]

The resulting function \( \lambda_k[E_{av}] \) is then used in equation (19).
The function $\lambda[Q,N]$ for the $N=12$ quantum spectrum represented by vertical lines. Long-dash magenta line: small-$p_k$ approximation (10) and (11); short-dash green line: mean-$\lambda$ approximation (20); thick solid red line: finite-$N$ corrected calculation based on equation (19) and section 3; thin solid black line: asymptotic behavior (20) and (21). Inset: normalization test of the mean-$\lambda$ approximation (dashed green line) and the finite-$N$ corrected calculation (solid red line).

Figure 1 presents curves for $\lambda[Q,N]$ obtained in various theoretical approximations. The numerical algorithms for computing these curves are described in the appendix. The calculations of all the three curves are based on satisfying the energy constraint (12). The small-$p_k$ approximation guarantees that the normalization constraint $\sum p_k$ is also satisfied [1]. However, the other approximations do not guarantee it a priori. Therefore, the check of the normalization constraint indicates the accuracy of the approximations. This check is presented in the inset of figure 1. It indicates that the normalization for the mean-$\lambda$ approximation falls short of 1 by about 10% (roughly 1/N), while for the finite-$N$ corrected calculation the deviation is about 1%.

Figure 2 presents a detailed comparison between Monte-Carlo results and the above analytical approximations for three different values of $Q$, 1.2, 1.4, and 1.6. The Monte-Carlo points accepted by the algorithm from [3] for the mean-$\lambda$ approximation are compared to the Monte-Carlo results. For $Q$ = 1.2, the mean-$\lambda$ approximation reproduces the Monte-Carlo results qualitatively, but with a large quantitative discrepancy, while the finite-$N$ corrected calculation is in good quantitative agreement with the Monte-Carlo results.

In the case of $Q = 1.6$, the Monte-Carlo result qualitatively corresponds to the prediction of [1] that, for macroscopic systems (meaning Gaussian density of states in the large-$N$ limit) at realistic positive Hilbert space temperatures $1/(N\lambda)$ (i.e. with $E_N < E_N^0$), the QMC ensemble leads to condensation into the lowest energy state with $P_1(p_1)$ having the character of $\delta$-function peaked at $\langle p_1 \rangle$, while all other states have small average occupations $\langle p_k \rangle$ and exhibit exponential shapes of $P_k(p_k)$. The Monte-Carlo results indicate that all $P_k(p_k)$ except $P_1(p_1)$ corresponding to the lowest spectral level $E_1 = -1.27$ have a nearly exponential shape well describable by all three of the approximations considered (figures 2(c) and (d)). The differences, however, become pronounced once $P_1(p_1)$ is considered. Figure 2(b) indicates that the small-$p_k$ approximation fails completely to describe $P_1(p_1)$, the mean-$\lambda$ approximation reproduces the Monte-Carlo results qualitatively, but with a large quantitative discrepancy, while the finite-$N$ corrected calculation is in good quantitative agreement with the Monte-Carlo results.

4. Numerical investigation of the QMC ensemble for a finite system

Here we compare analytical and numerical results for a quantum spectrum that has $N = 12$ energy levels. This is nearly the maximum number of quantum levels, whose statistics we can access in reasonable time with the Monte-Carlo algorithm described in [13]. The spectrum energies are $\{-1.27, -0.93, -0.68, -0.47, -0.27, -0.09, 0.09, 0.27, 0.47, 0.68, 0.93, 1.27\}$ shown in figure 1.
Figure 2. The results of a direct Monte-Carlo sampling of the QMC ensemble for the $N = 12$ quantum spectrum given in the text (blue circles) versus three analytical approximations based on functions $\lambda[E_{av}]$ presented in figure 1: magenta triangles and magenta long-dash lines: small-$p_k$ approximation (10) and (11); green diamonds and green small-dash line: mean-$\lambda$ approximation (20); red squares and red solid lines: finite-$N$ corrected calculation based on equation (19) and section 3.

The example of $E_{av} = 0$ corresponds to the infinite Hilbert space temperature. In this case, the small-$p_k$ approximation predicts that all $P_k(p_k)$ have the same exponential shape, and that, independently of $E_k$, $\langle p_k \rangle = 1/N$. This would indeed be the case in the limit $N \to \infty$. However, here the finite-$N$ corrections lead to a larger discrepancy with the Monte-Carlo results for all $k$. Two other approximations capture the above systematic trend, but the finite-$N$ corrected calculation exhibits better quantitative agreement.

The QMC ensemble implies a broad mixture of conventional thermal states, which, for a small subsystem, does not result in a single thermal BG distribution. The conclusion was confirmed by direct calculation in [1]. The author of [1] obtained analytically that the QMC-based density matrix for a small subsystem of an isolated macroscopic system is a weighed sum of two terms: the zero-temperature density matrix and the infinite temperature density matrix. In section 5, we present numerical evidence for a similar behavior of a finite-$N$ system.
5. Properties of a subsystem within a small spin system

In this section, we demonstrate numerically that the following qualitative property of the macroscopic limit also appears in the finite-\(N\) case. Namely, for a subsystem within an isolated quantum system, the lowest energy state and the states on the high-energy end of the spectrum have larger occupations for the QMC ensemble than for the canonical ensemble. Correspondingly, the intermediate energy states have smaller occupations for the QMC ensemble.

Below we consider a 12-level system consisting of two spins 1/2 and spin 1, and examine numerically the density matrix of the subsystem of two spins 1/2. As mentioned in the previous section, the 12-level limitation is due to the computational difficulty of sampling high-dimensional Hilbert spaces. We assume that the environment represented by spin 1 does not interact with the subsystem of two coupled spins 1/2. Hence the Hamiltonian of the entire system is \(H = H_I + H_S\), where

\[
H_I = y_I H_{1z} + I_{1x} I_{2x} + J_x I_{1y} I_{2y} + J_y I_{1z} I_{2z} \tag{31}
\]

and \(H_S = y_S H_S\) are, respectively, the Hamiltonians for the two spins 1/2 and for spin 1. Here \(I_{m\alpha}\) are the operators of the \(\alpha\)-components (\(\alpha = x, y, z\)) of the two spins 1/2 \((m = 1, 2)\), \(S_z\) is the operator of the z-component of spin 1, \(H = 3\) is the external magnetic field, and \(y_I = 0.7\) and \(y_S = 3\) are the gyromagnetic ratios for spins 1/2 and for spin 1, respectively; \(J_{x} = -2, J_{y} = -1, J_{z} = 0.5\) are anisotropic coupling constants. Since spin 1 plays the role of the environment, the parameters of the Hamiltonian were chosen such that the spread of the spin-1 levels is significantly larger than that of the two-spin-1/2 subsystem. The energy spectrum of the Hamiltonian \(H\) has three clearly identifiable four-level groups.

We compare the subsystem density matrices for the canonical ensemble \((T = 1)\) and the QMC ensemble at the same average energy of the entire system. The results on the diagonal elements of the density matrix \(\rho_{\alpha\alpha}\) in the eigenbasis of the Hamiltonian \(H_I\) are presented in figure 3. As expected from the large-\(N\) limit [1], the values of \(\rho_{\alpha\alpha}\) for the QMC ensemble are larger than those for the canonical ensemble for the lowest and highest subsystem energy levels and correspondingly smaller for the middle two levels.

If one has only limited experimental access to the properties of the subsystem, the QMC ensemble can be discriminated from the canonical ensemble by looking at the variance of the energies of the subsystem:

\[
(\Delta E_{\rho})^2 = \sum_{\alpha} \rho_{\alpha\alpha} (E_{\alpha} - \bar{E}_{\rho})^2, \tag{32}
\]

where index \(\alpha\) labels the subsystem’s eigenstates, \(E_{\alpha}\) denotes the corresponding subsystem eigenenergies, and \(\bar{E}_{\rho} = \sum_{\alpha} \rho_{\alpha\alpha} E_{\alpha}\) is the average energy of the subsystem. In figure 4, we plot subsystem energy variances for the QMC and the canonical ensembles as a function of \(\bar{E}_{\rho}\). For \(E_{\alpha\alpha} = E_1\) and \(E_{\alpha\alpha} = 0\), the predictions of the two ensembles are identical, and hence the variances are the same. Between \(E_{\alpha\alpha} = E_1\) and \(E_{\alpha\alpha} = E_0\), the energy variance of the QMC ensemble is always larger. This excessive energy variance can thus be used to identify the QMC ensemble experimentally.

6. Conclusions

In conclusion, we have demonstrated that the large-\(N\) analytical description of the QMC ensemble developed in [1] allows one to make good predictions on the Monte-Carlo sampling of the QMC ensemble for finite-\(N\) systems. The description in [1] is amenable to finite-\(N\) corrections, and once these corrections are introduced, it leads to accurate quantitative agreement with the Monte-Carlo results for systems with \(N \sim 10\).

We have also studied numerically the implications of the QMC ensemble for a subsystem of a small spin system. Our results indicate that, already in this rather artificial case, the behavior of the subsystem’s density matrix qualitatively follows the analytical result for the large-\(N\) case. We have further suggested that the energy variance of the subsystem can be used to discriminate experimentally between the QMC and the BG statistics.

Note added: When we were about to complete work on this paper, we became aware of a series of papers by Fresch and Moro [14–16] and by Wootters [17] very closely related to the scope of the present work and [1].
Appendix. Algorithms for finding $\lambda[E_v]$ and $\lambda_k[E_v]$

Here we describe the algorithm for finding $\lambda[E_v]$ from the mean-$\lambda$ integral equation (20)—‘Algorithm A’, and the modification of Algorithm A including finite-$N$ corrections based on equation (19) incorporating ansatz from section 3—‘Algorithm B’.

Function $\lambda[E_v]$ is defined in the interval $[E_{\text{min}}, E_{\text{max}}]$. We use a non-uniform discretization of this interval with 228 grid points—less dense in the middle and more dense near $E_{\text{min}}$ and $E_{\text{max}}$, where $\lambda[E_v]$ tends to diverge.

**Algorithm A**: The algorithm first finds $\lambda[E_v]$ in the small-$p_k$ approximation on the basis of equations (11) and (12) and then iteratively improves it by (i) calculating $V_k(p_k)$ by substituting $\lambda[E_v]$ into equation (20), (ii) finding the corresponding $\langle p_k \rangle$, (iii) checking the averaged energy condition (12) and (iv) improving the value $\lambda[E_v]$ by matching condition (12) and then returning to step (i). As explained below, step (iv) is done ‘locally’, i.e. for every $E_v$, on the grid it improves $\lambda[E_v]$ independently of the values of $\lambda[E_v]$ at other grid points, but then once all grid values of $\lambda[E_v]$ are improved, the algorithm returns to step (i) with the entire improved set of $\lambda[E_v]$.

In the small-$p_k$ limit, the algorithm for finding $\lambda[E_v]$ is ‘local’, i.e. it does not involve the explicit influence of $\lambda[E_v]$ at a given grid point on the average energy condition (12) at other grid points. In this case, the value of $\lambda$ is tried, and if it does not satisfy equation (12), then it is modified to $\lambda' = \lambda + \Delta \lambda$, which, according to equation (10), implies that $V_k(p_k)$ is also modified to become

$$V_k'(p_k) = V_k(0)e^{-Np_k[1+(\lambda+\Delta\lambda)(E_v-E_v)]}.$$  
(A.1)

This equation can now be rewritten as

$$V_k(p_k) = V_k(p_k)e^{-Np_k\Delta\lambda(E_v-E_v)}.  \hspace{1cm} (A.2)$$

In the above form, it amounts to a good approximation also to the case when $V_k(p_k)$ deviates from the exponential form. The calculated results presented in section 4 are based on six iterations involving equation (A.2).

**Algorithm B**: Algorithm A can now be modified to incorporate the finite-$N$ corrections associated with the deviations of individual functions $\lambda_k[E_v]$ from the ‘mean’ function $\lambda[E_v]$. Algorithm B continues searching for the mean function $\lambda[E_v]$, but at each step of Algorithm A that used equation (20), it uses equation (19) with the values of $\lambda_k[E_v]$ obtained from $\lambda[E_v]$ with the help of the ansatz described in section 3. The algorithm continues using the ‘local’ step involving equation (A.2).

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