Reduced-density-matrix spectrum and block entropy of permutationally invariant many-body systems

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Spectral properties of the reduced density matrix (RDM) of permutational invariant quantum many-body systems are investigated. The RDM block diagonalization which accounts for all symmetries of the Hamiltonian is achieved. The analytical expression of the RDM spectrum is provided for arbitrary parameters and rigorously proved in the thermodynamical limit. The existence of several sum rules and recurrence relations among RDM eigenvalues is also demonstrated and the distribution function of RDM eigenvalues (including degeneracies) characterized. In particular, we prove that the distribution function approaches a two-dimensional Gaussian in the limit of large subsystem sizes $n \gg 1$. As a physical application we discuss the von Neumann entropy (VNE) of a block of size n for a system of hard-core bosons on a complete graph, as a function of n and of the temperature T. The occurrence of a crossover of VNE from purely logarithmic behavior at $T=0$ to a purely linear behavior in n for $T \gtrsim T_c$, is demonstrated.

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I. INTRODUCTION

A great deal of interest is presently devoted to the study of the *entanglement* properties of interacting quantum many-body systems [1] due to their relevance for the newly developing technologies of quantum computation and quantum cryptography [2]. Entanglement represents a key resource for such fields because it provides information about how much correlations present in a quantum state can be used to control a quantum device [3,4]. This problem has been investigated for several interesting systems of condensed matter physics, including spin chains [5–13], Hubbard [8,14,15] and pairing models [16], itinerant bosonic systems [17], harmonic lattices [18], etc.

There are several different measures of entanglement, the most famous one being the so called *von Neumann entropy* (VNE) of a subsystem, also known as block or entanglement entropy [3]. At zero temperature the VNE provides a measure of the maximal compression rate of a quantum information in an ideal coding scheme. Recently, the VNE has been used to detect quantum phase transitions and topological vs quantum order, in strongly correlated systems [19,20].

The calculation of the entanglement entropy involves the knowledge of the so called *reduced density matrix* (RDM), a tool very useful to characterize quantum correlations. The RDM contains complete information about an open quantum system, i.e., a quantum systems in contact with its environment such as a thermal bath or another larger quantum system of which it constitutes a part. The spectrum of the RDM may reveal intrinsic, sometimes universal, properties of the subsystem through its link with the VNE.

For a subsystem of size n the RDM is a $2^n \times 2^n$ matrix and for large n the calculation of the spectrum becomes a problem of exponential growing difficulty. Explicit calculations of the VNE have been performed for a number of one-dimensional spin models [7–13,21,22]. Entanglement entropy for antiferromagnetic–ferromagnetic alternating Heisenberg chain has been investigated by density-matrix renormalization-group method in [23] and for large block of spins in the ground state of XY spin chain in [24].

Especially relevant appears the connection between entanglement entropy and quantum phase transitions [25]. In the case of the antiferromagnetic Heisenberg spin chain with anisotropy parameter, the VNE has been calculated in critical phases by using the conformal field symmetry which governs long-distance correlations in the system [8,26,27]. In this context it has been shown that at the quantum critical point the VNE for a subsystem of size n grows logarithmically with n, with an universal prefactor which is equal to the central charge of the underlying conformal field theory (CFT) [5,6,8,25,28].

Although a limiting distribution function can be calculated in the CFT case (see [29]) the analytic knowledge of the RDM spectrum is practically unknown, and up to date no analytical expressions of the RDM eigenvalues exist for generic interacting many body systems. To our knowledge, the full spectrum of the RDM for arbitrary sizes n of the subsystem has been calculated only for the very special case of non interacting particles (free fermions or free bosons), see, e.g., [30–32], or for small size subsystems (analytic expressions of the RDM for a subsystem of $n<6$ spins have been recently calculated for some special case of the antiferromagnetic XXZ chain of odd length [33]).

Entanglement properties of many-body systems at finite temperature have been investigated in [34]. The exact knowledge of the RDM spectrum for arbitrary sizes of the subsystem permits to study the thermodynamic properties of the VNE and allows to shed some light on the interplay between the quantum nature of the system and its thermodynamics [35]. In particular, the scaling law of the VNE across a finite temperature phase transition was recently investigated for a system of hard-core bosons in Ref. [35], where an analytical expression of the RDM spectrum was provided without any proof.

The aim of the present paper is to present a detailed investigation of the spectral properties of the RDM and VNE of permutational invariant quantum many-body systems. To this regard, we use the symmetry of the system to achieve the complete block diagonalization of the RDM. The analytical expression for the spectrum is provided for arbitrary parameters and rigorously proved in the thermodynamical limit. The existence of several sum rules and recurrence relations among RDM eigenvalues is also demonstrated. These rules are very useful for developments of the RDM spectral theory as well as for testing both analytical and numerical results. The existence of particle-hole symmetry at half filling is discussed and the distribution function of RDM eigenvalues (including degeneracies) characterized. In particular, we prove that the distribution function approaches a two-dimensional Gaussian in the limit of large subsystem sizes. As application, we consider the case of a system of N hard-core bosons on a full graph which undergo a Bose-Einstein condensation at $T=T_c$ [36,37]. The VNE entropy of a block of n hard-core bosons is computed as a function of n and of the temperature T and the occurrence of a crossover from a purely logarithmic behavior in n of the VNE at $T=0$, to a purely linear (extensive) behavior for $T\geq T_c$, is demonstrated.

The paper is organized as follows. In Sec. II, we introduce our model Hamiltonians for permutational invariant quantum many-body systems and give basic definitions to which our analysis applies. In Sec. III, we show how the Hamiltonian symmetries allow to block diagonalize the RDM for subsystems of arbitrary size. In Sec. IV, we discuss the implications of these symmetry properties on the eigenvalues of the RDM and show the existence of several sum rules for RDM eigenvalues. In Sec. V, we derive one step recursive relations among RDM eigenvalues which arise from the tracing out process of one site. Analytical expressions of the RDM eigenvalues for arbitrary parameter values are given in Sec. VI, a proof of which is provided in the thermodynamical limit. In Sec. VII, we show that the distribution function of the RDM eigenvalues approaches a Gaussian distribution in the limit of large block sizes. In Sec. VIII, we discuss properties of the von Neumann entropy for permutational invariant systems while in Sec. IX, we apply our results to the specific case of a system of hard-core bosons. For this case we discuss the dependence of the VNE on temperature and its scaling law across a phase transition to a Bose-Einstein condensate occurring at a finite temperature. Finally, in Sec. X, the main results of the paper are briefly summarized.

II. MODEL AND BASIC DEFINITIONS

Let us consider a system of hardcore bosons described by the following permutational invariant Hamiltonian

$$H = -\frac{1}{L}\sum_{i,j}^{L} b_i^{+}b_j + \sum_{i=1}^{L} b_i^{+}b_i, \tag{1}$$

where $b_i^{\dagger}, b_i$, denote creation and annihilation operators satisfying the deformed Heisenberg algebra: $[b_i,b_j]=0$, $[b_i^{+},b_j^{+}]=0$, and $[b_i,b_j^{+}]=(1-2b_j^{+}b_i)\delta_{ij}$ [37]. Due to the onsite Fermi-like commutation relations, double occupancy is not allowed: the action of b_i^{+} and b_i on the single particle Fock space being $b_i^{+}|0\rangle=|1\rangle$; $b_i|1\rangle=|0\rangle$; $b_i|0\rangle=b_i^{+}|1\rangle=0$. Using the transformation $S_k^{+}=S_k^{x}+iS_k^{y}=b_k^{+}/2$, $S_k^{-}=S_k^{x}-iS_k^{y}=b_k/2$, $S_k^{z}=1/2-b_k^{+}b_k$, the Hamiltonian Eq. (1) can be rewritten in terms of spin 1/2 operators as

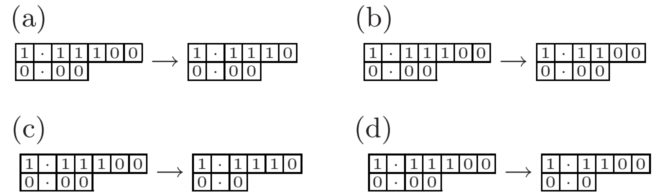

FIG. 1. Filled YTs involved in the one step reduction $\rho_n \rightarrow \rho_{n-1}$. Panels a),b), correspond to eigenvalues $\lambda_{n-1,k-p,s-q}^{n,k,s}$ with $q=0$ and $p=0$, $p=1$, respectively. Panels c),d), correspond to eigenvalues $\lambda_{n-1,k-p,s-q}^{n,k,s}$ with $q=1$ and $p=0$, $p=1$, respectively.

$$H = -\frac{1}{4L}[\mathbf{S}^2 - S^z(S^z-1)] + \left(\frac{L}{2} - S^z\right). \tag{2}$$

Here $\mathbf{S}\equiv(S^x,S^y,S^z)$, $S^{\alpha}=\frac{1}{2}\sum_{i=1}^{L}\sigma_i^{\alpha}$, with σ_i^{α} Pauli matrices acting on subspace i of the Hilbert space factorized as tensor product of L subspaces $\Pi_1^L\otimes C_2$. Note that H is invariant under the action of the symmetric group $\mathbf{S}_L$ and conserves the total spin polarization S^z, $[H,S^z]=0$ (in the language of hard-core bosons $S^z\equiv L-2N$, with $N=\sum_{i=1}^{L}b_i^{+}b_i$ the total number operator). We remark that besides these Hamiltonians, our results will apply to other models which are invariant under the action of the symmetric group S_L, such as the isotropic Lipkin-Meshkov-Glick (LMG) model [38,39], Curie-Weiss Hamiltonian, etc.

The unit vectors $|\Psi_{L,N,r}\rangle\subset\Pi_1^L\otimes C_2$, with N spins down (e.g., of polarization $(L-N)/2$), associated to filled Young tableaux (YT) of type $\{L-r,r\}_{(N)}$, form a complete set of eigenstates of H

$$H|\Psi_{L,N,r}\rangle = E_{L,N,r}|\Psi_{L,N,r}\rangle,$$

$$E_{L,N,r} = r + \frac{1}{L}(N(N-1) - r(r-1)),$$

$$S^z|\Psi_{L,N,r}\rangle = (L-2N)|\Psi_{L,N,r}\rangle. \tag{3}$$

Here and in the following we denote with the symbol $\{L-r,r\}_{(N)}$ a two rows YT with $L-r$ boxes (sites) in the first row and r in the second, filled with N quanta (N spins up, in the present context). Typical filled YTs are depicted in Fig. 1 (see [37] for more details). Note that $N=0,1,\ldots,L$ determines possible values of total spin polarization $(L-N)/2$ and r takes values $r=0,1,\ldots,\max(N,L-N)$. The degeneracy of an eigenvalue $E_{L,N,r}$ is given by the dimension of the respective YT, e.g.

$$\deg_{L,r} = \binom{L}{r} - \binom{L}{r-1}. \tag{4}$$

The global density matrix, $\varsigma_{L,N,r}$, (e.g., the density matrix of the full system=subsystem+environment) is defined as

$$\varsigma_{L,N,r} = \frac{1}{\deg_{L,r}} \sum_{u=1}^{\deg_{L,r}} |\Psi_u\rangle\langle\Psi_u| = \frac{1}{\deg_{L,r}} \sigma_{L,N,r} \tag{5}$$

with the set of vectors $|\Psi_u\rangle$, $u=1,\ldots \deg_{L,r}$, forming an orthonormal basis in the eigenspace of H with eigenvalue $E_{L,N,r}$. The matrix $\sigma_{L,N,r}$ acts on the Hilbert space $\Pi_1^L \otimes C_2$ and satisfies the following properties (see [40]):

(i) $\sigma_{L,N,r}$ has $\deg_{L,r}$ nonzero eigenvalues all equal to 1 and trace $\mathrm{Tr}\sigma_{L,N,r}=\deg_{L,r}$ equal to the dimension of the corresponding YT;

(ii) $(\sigma_{L,N,r})^2=\sigma_{L,N,r}$;

(iii) $[\sigma,P_{ij}]=0$ for any i,j, with P_{ij} operators permuting the subspaces i and j in the product $\Pi_1^L \otimes C_2$.

Our main interest is not on $\varsigma_{L,N,r}$ but on the RDM of a subsystem of n sites, ρ_n, obtained from $\varsigma_{L,N,r}$ by tracing out $L-n$ sites (degrees of freedom):

$$\rho_n = \mathrm{Tr}_{L-n} \varsigma_{L,N,r} \tag{6}$$

(for notational convenience the dependence of ρ_n on L,N,r will be omitted). Since ρ_n is a density matrix, its eigenvalues are real and nonnegative and its trace is equal to 1. Moreover, due to the property (iii), ρ_n does not depend on the particular choice of the n sites, and satisfies the property (iii) in its subspace: $[\rho_n, P_{ij}]=0$ for any i,j. In the following sections we discuss RDM properties which are directly linked to Hamiltonian symmetries.

III. RDM BLOCK DIAGONALIZATION

To characterize the spectral properties of the RDM we take advantage of the permutational invariance of the Hamiltonian by exploiting the decomposition of ρ_n into irreducible representations (irreps) of the symmetric $\mathbf{S}_n$ (permutation group of n objects). Let us consider an initial state associated to a Young tableau of $\mathbf{S}_L$ of type $\{L-r,r\}_{(N)}$ with $0<r\leq[L/2]$ where $[x]$ denotes the integer part of x. Note that, due to the symmetry and antisymmetry of a YT with respect to rows and columns, respectively, this state can exist only if $N\geq r$. After making trace with respect to $L-n$ sites one obtains states associated to filled YTs of $\mathbf{S}_n$ of type $\{n-s,s\}_{(k)}$ with $k=0,1,\ldots,n$ and $s=0,1,\ldots,k$. The conservation of the total spin polarization S^z (number of particles for hard-core bosons) implies that ρ_n has $n+1$ blocks B_k distinguished by the value of the spin polarization $(n-k)/2$. On the other hand, the invariance of the Hamiltonian under permutations implies that each block B_k can be further diagonalized into $k+1$ sub-blocks associated to filled YTs of type $\{n-s,s\}_{(k)}$ with s compatible with the filling, e.g., $s=0,1,\ldots,\min(k,n-k)$. Thus, for example, blocks B_0,B_1,B_2, etc. have the form

$$B_0 = \left(\begin{array}{|c|c|c|c|c|c|c|}\hline 0&\cdot&\cdot&\cdot&\cdot&\cdot&0\\\hline\end{array}\right)$$

$$B_1 = \begin{pmatrix} \begin{array}{|c|c|c|c|c|c|c|}\hline 1&0&\cdot&\cdot&\cdot&\cdot&0\\\hline\end{array} & \\ & \begin{array}{|c|c|c|c|c|c|}\hline 1&0&\cdot&\cdot&\cdot&0\\\hline \multicolumn{1}{|c|}{0}\\\cline{1-1}\end{array} \end{pmatrix}$$

$$B_2 = \begin{pmatrix} \begin{array}{|c|c|c|c|c|c|}\hline 1&1&0&\cdot&\cdot&0\\\hline\end{array} & & \\ & \begin{array}{|c|c|c|c|c|c|}\hline 1&1&0&\cdot&\cdot&0\\\hline \multicolumn{1}{|c|}{0}\\\cline{1-1}\end{array} & \\ & & \begin{array}{|c|c|c|c|c|}\hline 1&1&0&\cdot&0\\\hline 0&\multicolumn{1}{c|}{0}\\\cline{1-2}\end{array} \end{pmatrix}, \quad etc\ .,$$

where 1 and 0 in the YTs denote, respectively, spin up (particle) and spin down (hole) for spin models (respectively, hard-core bosons). The dimension of each block, $\dim(B_k)$, is given by the dimension of the Hilbert space of k spins up on n sites, e.g., $\binom{n}{k}$. Each filled YT of type $\{n-s,s\}_{(k)}$ in the block B_k contributes to the ρ_n spectrum with one degenerated eigenvalue whose degeneracy is equal to the dimension $\deg_{n,s}$ of the YT:

$$\deg_{n,s} = \binom{n}{s} - \binom{n}{s-1}.$$

Notice that the sum of the degeneracies of all eigenvalues of a block is equal to the dimension of the block

$$\dim(B_k) \equiv \sum_{s=0}^{k} \deg_{n,s} = \sum_{s=0}^{k} \binom{n}{s} - \binom{n}{s-1} = \binom{n}{k} \tag{7}$$

and the sum of the dimensions of all blocks appearing in ρ_n gives the full dimension of the Hilbert space

$$\sum_{k=0}^{n} \dim(B_k) = \sum_{k=0}^{n} \binom{n}{k} = 2^n.$$

These equalities show the consistency of the above block decomposition of the RDM. The fact that B_k is block diagonal with respect to the $\mathbf{S}_n$ irreps which are compatible with the filling k of the block, implies that the RDM ρ_n has the form

$$\rho_n = \sum_{k=0}^{n} B_k = \sum_{k=0}^{n} \sum_{s=0}^{\min(k,n-k)} B_{k,s} = \sum_{k=0}^{n} \sum_{s=0}^{\min(k,n-k)} \lambda_{n,k,s}^{L,N,r} \sigma_{n,k,s}, \tag{8}$$

where $B_{k,s}$ denote the sub-block $\{n,n-s\}_{(k)}$ of the block B_k spanned by the symmetrized basis

$$\sigma_{n,k,s} = \sum_{u=0}^{\deg_{n,s}} |nks,u\rangle\langle nsk,u|, \tag{9}$$

which accounts for the degeneracy $\deg_{n,s}$ of the ρ_n eigenvalue $\lambda_{n,k,s}^{L,N,r}$ with respect to $\{n-s,s\}_{(k)}$ states (here and in the following we denote the eigenvalues of ρ_n by $\lambda_{n,k,s}^{L,N,r}$ to display the full dependence on parameters).

IV. SUM RULES

The block diagonalization of the previous section implies a number of general properties for the spectrum of the RDM which can be presented in the form of the sum rules listed below.

(i) Sum rule with respect to s. The first sum rule can be derived by observing that

$$\mathrm{Tr}(B_k) = \sum_{s=0}^{\min(k,n-k)} \lambda_{n,k,s}^{L,N,r} \deg_{n,s} = w(B_k)\binom{n}{k}, \tag{10}$$

where $w(B_k)$ is the weight of the block

$$w(B_k) = \frac{\binom{L-n}{N-k}}{\binom{L}{N}}. \tag{11}$$

Note that $w(B_k)$ is just the correct probability factor one expects for states with k spins up on n sites obtained by eliminating $L-n$ sites and $N-k$ spins up from the initial state. The block weight $w(B_k)$, indeed, is just the ratio between the number of these states and the dimension $\binom{L}{N}$ of the whole Hilbert space for N spins up on L sites. Equations (10) and (11), then lead to the first sum rule for the eigenvalues

$$\sum_{s=0}^{\min(k,n-k)} \lambda_{n,k,s}^{L,N,r} \deg_{n,s} = \frac{\binom{L-n}{N-k}}{\binom{L}{N}} \binom{n}{k}. \tag{12}$$

It is worth to note that this expression is fully consistent with the normalization condition of ρ_n:

$$\mathrm{Tr}(\rho_n) = \sum_{k=0}^{n} \mathrm{Tr}(B_k) = \sum_{k=0}^{n} \frac{\binom{n}{k}\binom{L-n}{N-k}}{\binom{L}{N}} = 1.$$

From Eqs. (7) and (12), we infer that the eigenvalues must have the form

$$\lambda_{n,k,s}^{L,N,r} = w(B_k) \Lambda_{n,k,s}^{L,N,r}, \tag{13}$$

with $w(B_k)$ given by Eq. (11) and with $\Lambda_{n,k,s}^{L,N,r}$ denoting the weight of the sub-block $B_{k,s}$ (i.e., the number of different ways the states of the sub-block with fixed k and s can arise from a filled YT $\{L-r,r\}_N$ after tracing out $L-n$ sites and $N-k$ spin up). Notice that Eqs. (12) and (13), imply that the weights of the sub-blocks $B_{k,s}$ must satisfy the following normalization condition

$$\sum_{s=0}^{\min(k,n-k)} \Lambda_{n,k,s}^{L,N,r} \deg_{n,s} = \binom{n}{k}. \tag{14}$$

(ii) Sum rule with respect to k. A second sum rule can be derived by computing the splitting of a given irreps of $\mathbf{S}_L$ into irreps of $\mathbf{S}_n$ by using group's representation theory [41]. To this regard we remark that a representation $\{L-r,r\}$, which is irreducible for the group $\mathbf{S}_L$ is obviously reducible for its subgroup $\mathbf{S}_n$ and the problem of computing how many $\mathbf{S}_n$ states one gets from the original $\mathbf{S}_L$ state, arises. This amounts to compute the decomposition of the $\mathbf{S}_L$ irrep of type $\{L-r,r\}$ into irreps of $\mathbf{S}_n$ of type $\{n-s,s\}$, $0 \le s \le [n/2]$, a problem which is encountered in quantum mechanics in connection with the splitting of levels induced by a perturbation. The decomposition of an arbitrary representation of $\mathbf{S}_L$ with characters χ into irreps of $\mathbf{S}_n$ with characters χ^s, follows from the following property of group representation theory [41]

$$n_s = \frac{1}{R}\sum_{i=1}^{g} g_i (\chi_i^s)^* \chi_i,$$

where g is the number of different inequivalent irreps of $\mathbf{S}_n$, g_i the size of the ith conjugacy class and R the order of $\mathbf{S}_n$. For case of YTs with only two rows one can show that n_s is

$$n_s = \binom{L-n}{r-s} - \binom{L-n}{r+s-n-1}.$$

Notice that the splitting of the initial irreps $\{L-r,r\}$ implies that

$$\sum_{s=0}^{n} n_s \deg_{n,s} = \deg_{L,r}$$

and the block decomposition of the RDM implies that

$$\sum_{k=s}^{n-s} \lambda_{n,k,s}^{L,N,r} = \frac{n_s}{\deg_{L,r}} = \frac{\binom{L-n}{r-s} - \binom{L-n}{r+s-n-1}}{\deg_{L,r}}, \tag{15}$$

with $s=0,\ldots,[\frac{n}{2}]$. Equation (15) can be easily understood if one notice that by multiplying both sides by the degeneracy of the eigenvalue $\deg_{n,s}$ one obtains on the left hand side the sum of all the eigenvalues associated with a tableau of a given type $\{n-s,s\}$ and on the right hand side the number of states of symmetry $n-s,s$ divided by the number of states of symmetry $\{L-r,r\}$, this being just the correct weight one would expect from the splitting of the initial tableau $\{L-r,r\}$ into tableaux of type $\{n-s,s\}$. The sum rule is indeed a direct consequence of the splitting of the irreps of $\mathbf{S}_L$ into irreps of $\mathbf{S}_n$ discussed above.

As a simple application of Eq. (15), we can derive the analytical expression of the eigenvalues of the RDM corresponding to sub-block of the block $k=n/2$ belonging to the irreps $\{\frac{n}{2},\frac{n}{2}\}$ (we assume here n even). Since $k=n/2$ represents the maximal value of the filling permitted by the $\mathbf{S}_n$ symmetry, there exists only one filled YT of type $\{\frac{n+1}{2},\frac{n-1}{2}\}$ in the block decomposition of ρ_n. Equation (15) for $k=s=n/2$ then gives (see also case ii) of Appendix B):

$$\lambda_{n,n/2,n/2}^{L,N,r} = \frac{\binom{L-n}{r-\frac{n}{2}} - \binom{L-n}{r-\frac{n}{2}-1}}{\binom{L}{r} - \binom{L}{r-1}}. \tag{16}$$

(ii) Particle-hole exchange and sum rule with respect to N. We now discuss a general property of the RDM eigenvalues which is related to the exchange of spins up with spins down, a property which we also refer to as *particle-hole* exchange. This property allows to relate eigenvalues of the blocks B_k with the ones of the block B_{n-k} for fixed N,L,r,n,s, as well as, between N and $L-N$ eigenvalues for fixed L,r,r,s,k (these relations permits to reduce the computation of the spectrum up to half-filling). To this regard, we note that blocks B_k and B_{n-k} differ only for having the number of spin up and spin down exchanged. Since the dimensions of the Hilbert spaces of the blocks are the same, the equality of the normalization conditions implies the equalities of the corresponding weights in the blocks, e.g., weights must be invariant under the particle-hole exchange (e.g., $k \to n-k$):

$$\Lambda_{n,k,s}^{L,N,r} = \Lambda_{n,n-k,s}^{L,N,r}. \tag{17}$$

A similar equation is obtained when the particle-hole exchange is applied on the initial state (e.g., $N \to L-N$):

$$\Lambda_{n,k,s}^{L,N,r} = \Lambda_{n,k,s}^{L,L-N,r}. \tag{18}$$

From the last two equations we also get that $\lambda_{n,k,s}^{L,N,r} = \lambda_{n,n-k,s}^{L,L-N,r}$. These equalities, together with Eqs. (11) and (13), imply that eigenvalues of the block k with a fixed s,N are related to the ones of the block $n-k$ with for the same value of s, N, as well to eigenvalues with the same k, s, but with the initial number of particle N replaced by $L-N$, by the following relations:

$$\lambda_{n,n-k,s}^{L,N,r} = \frac{\binom{L-n}{N-n+k}}{\binom{L-n}{N-k}} \lambda_{n,k,s}^{L,N,r}, \tag{19}$$

$$\lambda_{n,k,s}^{L,L-N,r} = \frac{\binom{L-n}{L-N-k}}{\binom{L-n}{N-k}} \lambda_{n,k,s}^{L,N,r}. \tag{20}$$

Note from these equations that at half-fillings, i.e., for $k=n/2$ or $N=L/2$ or both, the particle-hole exchange introduces additional degeneracies in the RDM spectrum and becomes an exact symmetry of the system. Equations (19) and (20), together with the sum rule Eq. (15), can be used to derive the analytical expressions for the eigenvalues corresponding to the filled YTs of type $\{\frac{n+1}{2}, \frac{n-1}{2}\}$ (in this case n is odd). To this regard we remark that this $\mathbf{S}_n$ symmetry allows two values of the filling: $k=\frac{n-1}{2}$ and $k=\frac{n+1}{2}$, so that from Eq. (15) we get

$$\lambda_{n,n-1/2,n-1/2}^{L,N,r} + \lambda_{n,n+1/2,n-1/2}^{L,N,r} = \frac{\binom{L-n}{r-\frac{n-1}{2}} - \binom{L-n}{r+\frac{n-1}{2}-1}}{\deg_{L,r}}. \tag{21}$$

On the other hand from Eq. (19) we have

$$\lambda_{n,n+1/2,n-1/2}^{L,N,r} = \frac{\binom{L-n}{N-\frac{n+1}{2}}}{\binom{L-n}{N-\frac{n-1}{2}}} \lambda_{n,n-1/2,n-1/2}^{L,N,r}.$$

Substituting this expression into Eq. (21) we obtain

$$\lambda_{n,n-1/2,n-1/2}^{L,N,r} = \frac{2N-n-1}{2(L-n-1)} \frac{\binom{L-n}{r-\frac{n-1}{2}} - \binom{L-n}{r+\frac{n-1}{2}-1}}{\deg_{L,r}}.$$

For arbitrary fillings Eqs. (19) and (20) also allow to write the following general identities

$$\lambda_{n,k,s}^{L,L-N,r} = \lambda_{n,n-k,s}^{L,N,r}.$$

From this equation we see that eigenvalues of the reduced density matrices ρ_n for N initial particles coincide with the ones of $L-N$ initial particles up to an exchange of particles with holes ($k \leftrightarrow n-k$). In view of these equalities the average with respect to the filling of the eigenvalues of ρ_n associated with a YT of type $\{n-s,s\}$ can be computed equivalently in two different manner, e.g., either with respect to N, for fixed L,r,n,k, or with respect to k, for fixed L,N,r,n, e.g.,

$$\frac{1}{L-2r+1} \sum_{N=r}^{L-r} \lambda_{n,k,s}^{L,N,r} = \frac{1}{n-2s+1} \sum_{k=s}^{n-s} \lambda_{n,k,s}^{L,N,r}.$$

Substitution of Eq. (15) in the right hand side of the above equation leads to the sum rule of the RDM eigenvalues with respect to N

$$\sum_{N=r}^{L-r} \lambda_{n,k,s}^{L,N,r} = \frac{L-2r+1}{n-2s+1} \frac{\binom{L-n}{r-s} - \binom{L-n}{r+s-n-1}}{\deg_{L,r}}. \tag{22}$$

V. ONE STEP RDM REDUCTION

In this section, we discuss recursion relations which allow to link eigenvalues of ρ_{n-m} to those of ρ_n for arbitrary n and m. In this respect, we consider the one step reduction $\rho_n = \mathfrak{s}_{n,k,s} \to \rho_{n-1} = \mathrm{Tr}_1(\rho_n)$. After tracing out one site we obtain

$$\mathrm{Tr}_1(\mathfrak{s}_{n,k,s}) = \sum_{\substack{p=0,1\\q=0,1}} \lambda_{n-1,k-p,s-q}^{n,k,s} \sigma_{n-1,k-p,s-q}, \tag{23}$$

with $\sigma_{n,k,s}$ given by Eq. (9). Note that the eigenvalues at the initial step are given by $\lambda_{n,k',s'}^{n,k,s} = 1/\deg_{n,s} \delta_{k,k'} \delta_{s,s'}$ and that after a single trace operation the numbers k',s', can decrease at most by one unity. Moreover, from $\mathrm{Tr}(\rho_{n-1,k,s})=1$ we have

$$\sum_{\substack{p=0,1\\q=0,1}} \deg_{n-1,s-q} \lambda_{n-1,k-p,s-q}^{n,k,s} = 1. \tag{24}$$

One can show (see Appendix A) that the eigenvalues involved in the one step reduction of the RDM are given by

$$\lambda_{n-1,k-p,s-q}^{n,k,s} \deg_{n-1,s-q} = \begin{cases} \frac{\deg_{n-1,s}}{\deg_{n,s}} \frac{n-s-k}{n-2s} & \text{if } \begin{matrix} p=0 \\ q=0 \end{matrix}, \\ \frac{\deg_{n-1,s}}{\deg_{n,s}} \frac{k-s}{n-2s} & \text{if } \begin{matrix} p=1 \\ q=0 \end{matrix}, \\ \frac{\deg_{n-1,s-1}}{\deg_{n,s}} \frac{k-s+1}{n-2s+2} & \text{if } \begin{matrix} p=0 \\ q=1 \end{matrix}, \\ \frac{\deg_{n-1,s-1}}{\deg_{n,s}} \frac{n-k-s+1}{n-2s+2} & \text{if } \begin{matrix} p=1 \\ q=1 \end{matrix}. \end{cases} \tag{25}$$

Schematically, one step reduction is depicted in Fig. 1. Relations Eq. (25) imply the existence of recursive relations among the eigenvalues of the RDMs which can be determined as follows. A link between ρ_n and ρ_{n-1} can be obtained by noting that from Eq. (8) ρ_n can be written as

$$\rho_n = \sum_{k,s} \lambda_{n,k,s}\sigma_{n,k,s} = \sum_{k,s} \lambda_{n,k,s}\, \mathrm{deg}_{n,s}\, \sigma_{n,k,s}, \tag{26}$$

where we introduced $\lambda_{n,k,s}$ as a shortcut notation for $\lambda_{n,k,s}^{L,N,r}$. The RDM ρ_{n-1} is obtained from ρ_n by tracing out one site from it, using Eq. (23), as

$$\rho_{n-1} = \mathrm{Tr}_1(\rho_n) = \sum_{k,s} \lambda_{n,k,s}\mathrm{Tr}_1(\sigma_{n,k,s})$$
$$= \sum_{k,s} \lambda_{n,k,s}\, \mathrm{deg}_{n,s} \sum_{\substack{p=0,1\\q=0,1}} \lambda_{n-1,k-p,s-q}^{n,k,s}\sigma_{n-1,k-p,s-q},$$

with $\lambda_{n-1,k-p,s-q}^{n,k,s}$ given by Eq. (25). Changing the order of the summations and rescaling indices k and s by p and q, respectively, we obtain

$$\rho_{n-1} = \sum_{k,s} \sum_{\substack{p=0,1\\q=0,1}} \lambda_{n,k+p,s+q}\, \mathrm{deg}_{n,s+q}\, \lambda_{n-1,k,s}^{n,k+p,s+q}\sigma_{n-1,k,s}.$$

On the other hand, from Eq. (26) ρ_{n-1} is also given by $\rho_{n-1}=\Sigma_{k,s}\lambda_{n-1,k,s}\sigma_{n-1,k,s}$ and a comparison with the above expression gives

$$\lambda_{n-1,k,s} = \sum_{\substack{p=0,1\\q=0,1}} \mathrm{deg}_{n,s+q}\, \lambda_{n-1,k,s}^{n,k+p,s+q}\lambda_{n,k+p,s+q}$$

for any k,s. By substituting the eigenvalues $\lambda_{n-1,k,s}^{n,k+p,s+q}$ from Eq. (25) we obtain the following recurrence relation for the RDM eigenvalues:

$$\begin{aligned}(n-2s)\lambda_{n-1,k,s} &= (n-s-k)\lambda_{n,k,s} + (k-s)\lambda_{n,k,s+1}\\ &\quad + (k+1-s)\lambda_{n,k+1,s}\\ &\quad + (n-k-s-1)\lambda_{n,k+1,s+1}.\end{aligned} \tag{27}$$

This equation allows a complete determination of all RDM eigenvalues. Indeed the recursive application of Eq. (27) to the initial global density matrix eigenvalues for L sites Eq. (5), which are known due to property (i) in Sec. II, generates all other eigenvalues for the RDM ρ_n for $n=L-1,L-2,\ldots$ etc. down to $n=1$. We remark that ascending relations (e.g., from $n\to n+1\to\ldots L$) for RDM eigenvalues can also be derived by using, in addition to Eq. (27), extra relations coming from the sum rule Eq. (12), these allowing to solve for a complete set of algebraic equations for all step-up eigenvalues (we omit details for brevity).

VI. RDM EIGENVALUES

The results of this section are summarized by the following statement about the analytical expression of the RDM eigenvalues:

The eigenvalues of the reduced density matrix ρ_n of the eigenstates of H with N particles belonging to the irreps of $\mathbf{S}_L$ characterized by YTs of type $\{L-r,r\}$, with $r \le \min(N,[L-N])$ are given by

$$\begin{aligned}\lambda_{n,k,s}^{L,N,r} &= \frac{\binom{L-n}{N-k}}{\binom{L}{N}} \sum_{i=0}^{k-s} \binom{k-s}{i}\binom{n-k-s}{i}\\ &\quad\times \sum_{j=0}^{k-i} (-1)^j \frac{\binom{s}{j}}{\binom{L-N}{j+i}\binom{N}{j+i}}\\ &\quad\times \sum_{m=0}^{j+i} (-1)^m \binom{L-N-r}{j+i-m}\binom{N-r}{j+i-m}\binom{r}{m},\end{aligned} \tag{28}$$

with $k,s,$ quantum numbers taking the values $k=0,1,\ldots,\min(n,N)$, and $s=0,1,\ldots,\min(k,n-k)$. The corresponding degeneracies are given by $\mathrm{deg}_{n,s}=\binom{n}{s}-\binom{n}{s-1}$.

Equation (28) was given also in [35] without a proof. Here, we remark that it satisfies all properties derived in the previous section as one can easily check by using a symbolic program. In particular, Eq. (28) satisfies the one step recurrence relation Eq. (27) from which the full RDM spectrum can be obtained (by iterations) for arbitrary parameter values. In the following we provide a proof of this fact in the thermodynamic limit, e.g., when the system size L gets infinitely large $L\to\infty$, but the ratios N/L, r/L remain finite:

$$\lim_{L\to\infty}\frac{N}{L} = p, \quad \lim_{L\to\infty}\frac{r}{L} = \mu. \tag{29}$$

This limit is particularly important for characterizing the existence of phase transitions. In our case, the infinite system described by the Hamiltonian Eq. (1) undergoes a Bose-Einstein condensation at finite temperature T_c (see Sec. IX). In the thermodynamic limit the RDM eigenvalues Eq. (28) simplify to (see Appendix B)

$$\lambda_{n,k,s}^{p,\mu} = p^{n-k}q^k(1-\eta)^s \sum_{i=0}^{k-s} \eta^i \binom{k-s}{i}\binom{n-k-s}{i}, \tag{30}$$

$$= p^{n-k}q^k(1-\eta)^s {}_2F_1(-k+s,k-n+s;1;\eta), \tag{31}$$

where ${}_2F_1(a,b;c;z)$ is the Gauss hypergeometric function, $\lambda_{n,k,s}^{p,\mu} \equiv \lim_{L\to\infty}\lambda_{n,k,s}^{L,N,r}$, $q=1-p$ and the new parameter η is given by

$$\eta = \frac{(p-\mu)(q-\mu)}{pq}. \tag{32}$$

Substituting Eq. (31) into Eq. (27) and dividing by $p^{n-k-1}q^k(1-\eta)^s$ we have that the recursion relation in the thermodynamic limit becomes

$$\begin{aligned}(a+b)F_{a,b+1} &= bpF_{a,b} + (a-1)qF_{a-1,b+1} + ap(1-\eta)F_{a+1,b+1}\\ &\quad + (b+1)q(1-\eta)F_{a,b+2},\end{aligned} \tag{33}$$

where $F_{a,b+1}$ is a shorthand notation for ${}_2F_1(a,b;1;\eta)$ with $a=-k+s$ and $b=k+s-n$. Notice that in the context of the RDM spectrum, a and b in Eq. (33) are negative integers and the hypergeometric sum has always a finite number of terms Eq. (30). Equation (33), however, is valid for arbitrary a,b, i.e., for generic infinite hypergeometric series within their convergence radius. The proof of Eq. (33) follows from the Gauss contiguous relation between hypergeometric functions [44]

$$(b-c)_2F_1(a,b-1;c;\eta)+a(1-\eta)_2F_1(a+1,b;c;\eta)$$
$$=(a+b-c)_2F_1(a,b;c;\eta), \tag{34}$$

from which the following two identities are obtained:

$$(a+b)F_{a,b+1}=bF_{a,b}+a(1-\eta)F_{a+1,b+1},$$

$$(a+b-1)F_{a,b}=(a-1)F_{a-1,b}+b(1-\eta)F_{a,b+1}.$$

Note that the first identity follows by substituting $c=1$ and $b\to b+1$ in Eq. (34), while the second identity follows by setting $c=1$ in Eq. (34), interchanging a and b and using the symmetry of ${}_2F_1$ with respect to the first two arguments. By shifting the argument $b\to b+1$ in the second identity, and substituting them into Eq. (33) we have that the right-hand side of this equation becomes $(p+q)(a+b)F_{a,b+1}$ and, since $p+q=1$, it coincides with the left hand side. This concludes the proof of Eq. (28) in the thermodynamic limit.

In Fig. 2, we have depicted the spectrum of the RDM obtained from Eq. (28) for the case $n=6$, $L\to\infty$ and compared it with the limiting expression Eq. (30) for different values of the p. We also remark that for the limiting case $\mu=0$, $\eta=1$ Eq. (30) reproduces the result $\lambda_{n,k}=p^{n-k}q^k\binom{n}{k}$ obtained in [12].

VII. SPECTRAL DISTRIBUTION FUNCTION

In this section we characterize the distribution function of the RDM eigenvalues in the limit of large subsystem sizes n. In particular, we show that the following statement is valid:

The distribution function of the RDM eigenvalues Eq. (30) taken with their degeneracies, $Q(k,s)=\lambda^{p,\eta}_{n,k,s}\,\deg_{n,s}$, in the limit of large n ($n\gg 1$) asymptotically approaches the two-dimensional Gaussian distribution with mean $\langle k/n\rangle=q$, $\langle s/n\rangle=\mu$:

$$Q(k,s)\approx Q_{\max}e^{-[(s-n\mu)^2/2C+(k-nq)^2/2D+(s-n\mu)(k-nq)/B]}, \tag{35}$$

with

$$Q_{\max}=\frac{1-2\mu}{2\pi n\sqrt{\mu(1-\mu)(p-\mu)(q-\mu)}},$$

$$B^{-1}=\frac{(1-2\mu)(p-q)}{n(p-\mu)(q-\mu)},\quad D^{-1}=\frac{(1-2\mu)^2}{n(p-\mu)(q-\mu)}, \tag{36}$$

$$C^{-1}=\frac{1}{n\mu(1-\mu)}+\frac{(p-q)^2}{n(p-\mu)(q-\mu)}. \tag{37}$$

We split the proof of this statement into two parts: in the first part we show that the maximum of Q occurs at the point $[k_{\max}/n=q+O(\frac{1}{n}),s_{\max}/n=\mu+O(\frac{1}{n})]$ while in the second one we evaluate the amplitude $Q_{\max}=Q(k_{\max},s_{\max})$ and the behavior of Q around the maximum. The first part, being more technical, is relegated to Appendix C and assumed for granted in the following. We also fix parameters p,η, as in Eqs. (29) and (32) and concentrate on the dependence of Q on parameters $k/n,s/n$, assuming $n\gg 1$, neglecting all finite size corrections of order $O(\frac{1}{n})$. Using the thermodynamic expression of the eigenvalues in Eq. (30), we write Q in the form

$$Q(k,s)=P\sum_{i=0}^{k-s}\eta^i\binom{M}{i}\binom{K}{i} \tag{38}$$

with $M=k-s$, $K=n-k-s$ and P given by

$$P=p^{n-k}q^k(1-\eta)^s\deg_{n,s}=\binom{n}{s}\frac{n-2s+1}{n-s+1}p^{n-k}q^k(1-\eta)^s. \tag{39}$$

To evaluate the amplitude $Q_{\max}$ and the behavior of $Q(k/n,s/n)$ around this point, we use the well known Gaussian approximation of the binomial distribution

$$\binom{Z}{i}\beta^i\alpha^{Z-i}\approx\frac{1}{\sqrt{2\pi\sigma^2}}\exp\left[-\frac{(i-Z\beta)^2}{2\sigma^2}\right],$$

with $0<\alpha=1-\beta<1$ and $\sigma^2=Z\alpha\beta\gg 1$, together with the fact (proven in Appendix C) that the major contribution to the sum in Eq. (38) for $k=k_{\max}$, $s=s_{\max}$, is obtained for $i=i_{\max}$ given by Eq. (C4). This allows to approximate the sum in Eq. (38) as

$$\sum_{i=0}^{k-s}\eta^i\xi_i\binom{M_0}{i}\alpha^i\beta^{M_0-i}\binom{K_0}{i}\gamma^i\delta^{K_0-i}$$
$$\approx\sum_{i=0}^{k-s}\frac{\eta^i\xi_i}{\sqrt{2\pi\sigma_{M_0}^2}\sqrt{2\pi\sigma_{K_0}^2}}e^{-(i-M_0\alpha)^2/2\sigma_{M_0}^2}e^{-(i-K_0\gamma)^2/2\sigma_{K_0}^2}, \tag{40}$$

with $\xi_i=1/(\alpha^i\beta^{M_0-i}\gamma^i\delta^{K_0-i})$, $\sigma_{M_0}^2=M_0\alpha\beta\gg 1$, $\sigma_{K_0}^2=K_0\gamma\delta\gg 1$, and M_0, K_0, α, β, γ, and δ given in Appendix C Using Eq. (32) we find that the term

$$\eta^i\xi_i=\frac{(1-\mu)^{M_0+K_0-2i}}{p^{K_0-i}q^{M_0-i}}\left[\frac{(p-\mu)(q-\mu)(1-\mu)^i}{pq(q-\mu)(p-\mu)}\right]^i$$
$$=\frac{(1-\mu)^{K_0+M_0}}{p^{K_0}q^{M_0}}=\frac{(1-\mu)^{n(1-2\mu)}}{p^{n(p-\mu)}q^{n(q-\mu)}}$$

does not depend on i, so that the sum Eq. (40) can be approximated with an integral (use $\sum_{i=0}^{k-s}\ldots\approx n\int_0^{q-\mu}\ldots dx$) as

$$n\int_0^{q-\mu}\frac{e^{-(i-M_0\alpha)^2/2\sigma_{M_0}^2}e^{-(i-K_0\gamma)^2/2\sigma_{K_0}^2}}{\sqrt{2\pi\sigma_{M_0}^2}\sqrt{2\pi\sigma_{K_0}^2}}dx=\frac{1}{\sqrt{2\pi n\frac{(p-\mu)(q-\mu)}{(1-\mu)(1-\mu)}}},$$

where in the last step we used the fact that since $x_m=(p-\mu)(q-\mu)/(1-\mu)$ is inside the segment $[0,q-\mu]$, for $n\gg 1$ the integration interval can be extended to the whole real axis. Collecting terms together, we have

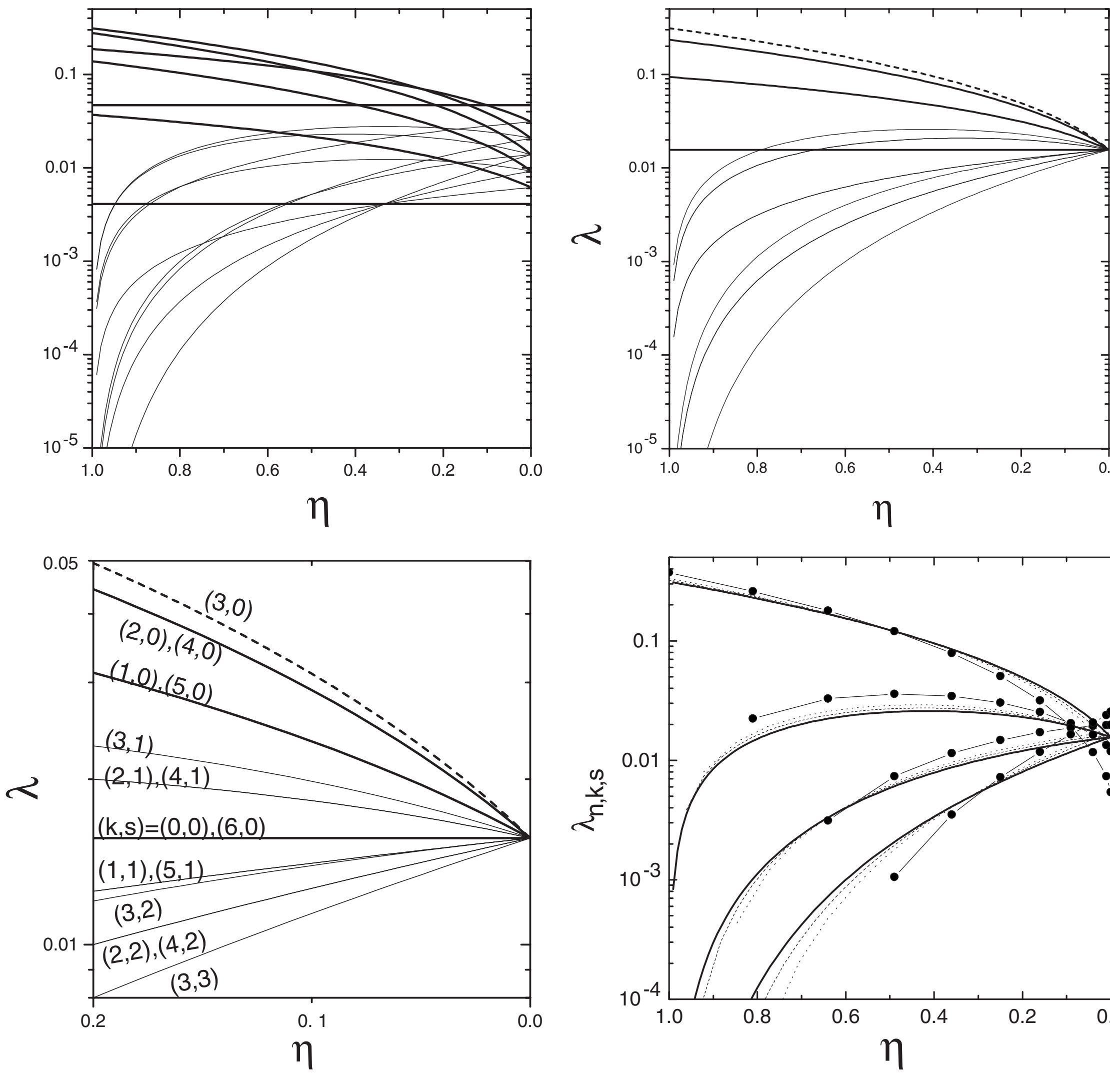

FIG. 2. Top Left panel. Eigenvalues Eq. (30) of the density matrix as function of η, for $n=6$, $L\to\infty$, $p=0.4$. Thick lines show the $(n+1)$ eigenvalues with $s=0$ which survive at $\mu=0$ (the remaining 2^n-n-1 eigenvalues vanish in this limit). Top Right Panel. The same as in the top left panel but for $p=0.5$ (half filling). Thick lines show n eigenvalues with $s=0$ (each being double degenerate), and the thick broken line shows the *only* nondegenerate eigenvalue with $k=3$, $s=0$. The number of different curves is reduced to $n/2+1$ due to the particle-hole symmetry Eq. (18) present at half-filling. Bottom Left Panel. Close up of the top right panel. Pairs of numbers (k,s) mark different eigenvalues $\lambda_{k,s}$. All eigenvalues have an additional degeneracy (due to particle-hole symmetry) except those of the block $k=3$. Bottom Right Panel. Comparison of the eigenvalues for finite and infinite L, for $n=6$: shown are the RDM eigenvalues of the block $k=3$ and $s=0,1,2,3$ (groups of curves from top to bottom). Solid lines correspond to the thermodynamic limit 30), while circles, dotted and dashed lines correspond to $L=10$, 50, and 100 [Eq. (28)], respectively. Parameters: $p=0.5$.

$$\sum_{i=0}^{k_{\max}-s_{\max}} \eta^i \binom{M_0}{i}\binom{K_0}{i} \approx \frac{(1-\mu)^{n(1-2\mu)}}{p^{n(p-\mu)}q^{n(q-\mu)}\sqrt{2\pi n\frac{(p-\mu)(q-\mu)}{(1-\mu)(1-\mu)}}}.$$

Equation (36) follows by substituting the above expression with $k_{\max}=nq$, $s_{\max}=n\mu$ in the definition of Q and using Stirling formula for $\deg_{n,s}$. Assuming that the behavior of $Q(k,s)$ in proximity of the maximum can be approximated by the equation obtained from Eq. (C6) by removing the point evaluation and integrating, we get Eq. (35) with the coefficients given by Eq. (37). For consistency we check that the above expression of Q leads to the correct normalization of ρ, e.g., $\mathrm{Tr}(\rho)=\Sigma Q(k,s)=1$. Using the identity $\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\exp(-\frac{1}{2}\Sigma A_{ij}x_ix_j)=2\pi/\det(A)$ and the expressions Eqs. (36) and (37), we get

$$\mathrm{Tr}(\rho) = \sum Q(k,s) = n^2\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} Q(nx,ny)dxdy$$

$$= Q_{\max}\frac{2\pi}{n^2\sqrt{CD-B^2}} = 1.$$

This conclude the proof of Eq. (35).

VIII. VON-NEUMANN ENTROPY

The exact knowledge of the RDM spectrum allows to calculate the von Neumann entropy as

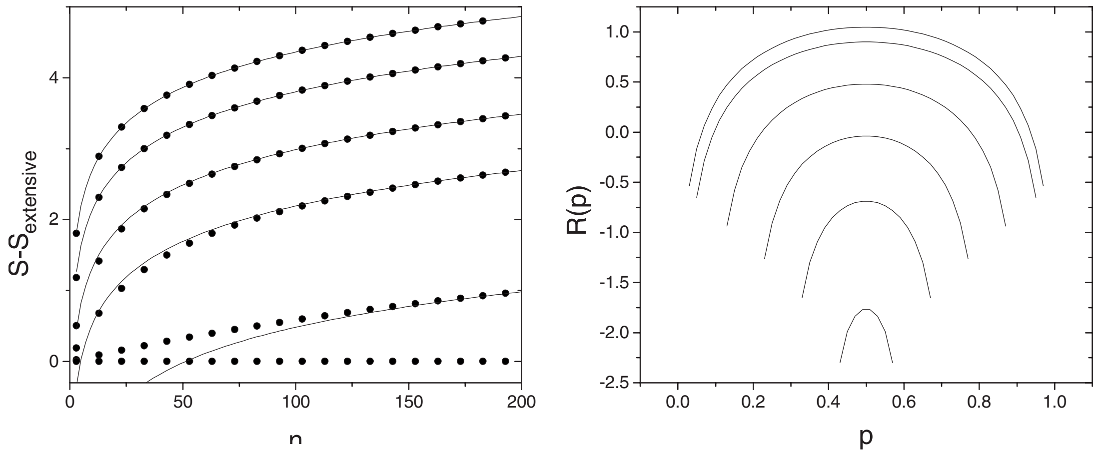

FIG. 3. Left: Von Neumann entropy in the thermodynamic limit, as function of n for $p=0.5$, and different μ. Data sets (top to bottom) correspond to $\mu/p=0.001$, 0.2, 0.5, 0.7, 0.9, and 0.999. Continuous curves correspond to the analytic prediction Eq. (42) with R as fitting parameter while dots refer to direct calculations of VNE using the exact expressions of the RDM eigenvalues. Right: Behavior of $R(p,\mu)$ in Eq. (42) as a function of p for different $\mu=0$, 0.02, 0.1, 0.2, 0.3, and 0.4 (data sets from top to bottom).

$$S_{(n)} = -\operatorname{Tr}(\rho_n \log \rho_n) = -\sum \deg_{k,s} \lambda^{L,N,r}_{n,k,s} \log \lambda^{L,N,r}_{n,k,s}.$$

It is instructive to investigate the thermodynamic limit of large $n \gg 1$ and infinite L, for which we can use the approximation Eq. (35). We obtain (see [35] for details)

$$S_{(n)} = -\sum_{k=0}^{n} \sum_{s=0}^{\min(k,n-k)} Q(k,s)\log_2 \frac{Q(k,s)}{\deg \lambda_{ks}}. \tag{41}$$

Substituting the sums with the integrals and using the normalization $\Sigma Q(k,s)=1$ and Eq. (35), we obtain

$$S_{(n)} \approx -n[\mu \log_2 \mu - (1-\mu)\log_2(1-\mu)] + \frac{1}{2}\log_2 n + R(p,\mu) \tag{42}$$

with $R(p,\mu)$ a smoothly varying function of p,μ (see right panel of Fig. 3). For special cases for which Eq. (35) cannot be applied, $S_{(n)}$ is given by different expressions (see subsection below). It is interesting to note that the extensive term, which gives the major contribution in the large n limit, coincides with the Boltzmann microcanonical entropy obtained in the limit $L\to\infty$, $r/L\to\mu$, as

$$\lim_{n\to\infty} \frac{S_{(n)}}{n} = \lim_{L\to\infty} \frac{1}{L}\log(\deg_{L,r}) \tag{43}$$

$$= \mu \log_2 \mu - (1-\mu)\log_2(1-\mu). \tag{44}$$

Here we have used the Stirling formula to estimate the degeneracy of eigenvalues as $\deg_{L,r} \approx \frac{1-2\mu}{(1-\mu)^{L-r+1}\mu^r}$.

In Fig. 3 we compare the VNE obtained by using the exact expressions of the RDM eigenvalues in Eq. (28) with the one obtained in the thermodynamic limit as function of n for different values of μ/p using the constant $R(p,\mu)$ in Eq. (42) as fitting parameter. In the right panel of this figure the dependence of $R(p,\mu)$ on p for different values of μ is depicted. Note that for given μ, the const R has its maximum at $p=0.5$ and is symmetric around this value with p allowed to vary from μ to $1-\mu$, this being a consequence of the particle-hole symmetry. Also note that the estimate Eq. (35) diverges in the points $\mu=0$, and $(p-\mu)(q-\mu)=0$ [see Eq. (36)]. These special cases are therefore considered separately below.

(i) Case $\mu=\lim_{L\to\infty}\frac{r}{L}=0$. Here we shall consider the extremal case, $r=0$, for which the state of the large system is a pure symmetric state. For $r=0$, and finite L, the RDM spectrum for ρ_n consists of only $n+1$ nonzero nondegenerate eigenvalues and is given by the hypergeometric distribution $\lambda^{L,N,0}_{n,k,s}=\delta_{s,0}\binom{n}{k}\binom{L-n}{N-k}/\binom{L}{N}$. In the thermodynamic limit Eq. (29) it becomes (we omit here index $s=0$ for brevity) $\lambda_k=q^k p^{n-k}\binom{n}{k}$. The von-Neumann entropy is readily calculated, noting that for $npq \gg 1$

$$\lambda_k \approx \frac{1}{\sqrt{2\pi npq}} \exp\left[-\frac{(k-nq)^2}{2npq}\right].$$

Replacing the sum $\Sigma\lambda_k \log_2 \lambda_k$ with the integral over real axis, we obtain

$$S_{(n)} = \frac{1}{2}\log_2 n + \frac{1}{2}\log_2 2\pi epq. \tag{45}$$

In the finite system of size L, the first term in the above will be replaced by $\frac{1}{2}\log_2\frac{n(L-n)}{L}$, see [12]. Note also that for symmetric states leading to the von Neumann entropy Eq. (45), other measures of entanglement, related to the distance to the closest separable state, can also be computed [42,43].

(ii) Case $(p-\mu)(q-\mu)=0$. Because of the particle-hole symmetry, it is enough to consider the case $p-\mu=\lim\frac{N-r}{L}=0$. Also here we shall consider the extremal case $N=r$, and start from finite system of size L. For $N=r$ the eigenvalues of the block k do not depend on s and are given by

$$\lambda_{n,k,s}^{L,N,r=N} = \frac{\binom{L-n}{N-k}}{\binom{L}{N}}.$$

In the thermodynamic limit we have $\lambda_{k,s}=q^k p^{n-k}$. Since the eigenvalues do not depend on s, each eigenvalue $q^k p^{n-k}$ has degeneracy $\binom{n}{k}$. The VNE then is (note that $\mu=\min(p,q)$)

$$S_{(n)} = -\sum_{k=0}^{n} \binom{n}{k} q^k p^{n-k} \log_2 q^k p^{n-k}$$
$$= n[\mu \log_2 \mu - (1-\mu)\log_2(1-\mu)], \qquad (46)$$

the sum being exact for arbitrary n.

IX. APPLICATION TO HARDCORE BOSONS

As an application of the above results in this section we discuss the VNE as a function of the temperature for a system of hard-core bosons described by the Hamiltonian Eq. (1). Our interest in this system resides in the fact that it exhibits a phase transition to a Bose-Einstein condensate (BEC) of hard-core bosons at $T=T_c\neq 0$ [36,37]. The above RDM analytical results provide a nearly unique opportunity to investigate the interplay between quantum and thermodynamical properties. This problem has been also recently investigated in [35] to which we refer for details.

The occurrence of a Bose-Einstein condensation in this system can be inferred directly from the free energy per site $F/L=\Lambda_{\min}/\beta$ where

$$\Lambda_{\min} = \beta p^2 + \min_{\mu\in[0,\min(p,q)]} \times [\beta\mu(1-\mu) + \mu \log \mu + (1-\mu)\log(1-\mu)], \qquad (47)$$

up to corrections of the order $O(L^{-1})$. The extremum condition for $\Lambda_{\min}$ leads to the equation

$$\beta^*(\mu^*) = \frac{1}{(1-2\mu^*)} \ln\left(\frac{1-\mu^*}{\mu^*}\right), \qquad (48)$$

This expression shows the existence of a phase transition to BEC at $T_c(p)=[\beta^*(p)]^{-1}$, with the density of particles in the condensate phase given by [36]

$$\rho_c = [p-\mu^*(\beta)][q-\mu^*(\beta)] \qquad (49)$$

below T_c and $\rho_c=0$ above T_c (see Fig. 4). Remarkably, the rescaled condensate density, $\rho_c/(pq)$, playing the role of order parameter which changes from 1 at $T=0$ to 0 at $T=T_c$, is equal to the parameter η in Eq. (32) which determines RDM eigenvalues [see Eq. (31), e.g., we have that $\rho_c/(pq)=\eta$].

To characterize the scaling law of the VNE across the phase transition to hard-core BEC, we consider the thermal VNE for a block of size n defined as

$$S_{(n)}(\beta) = \mathrm{Tr}[\rho_n(\beta)\log_2 \rho_n(\beta)], \qquad (50)$$

where

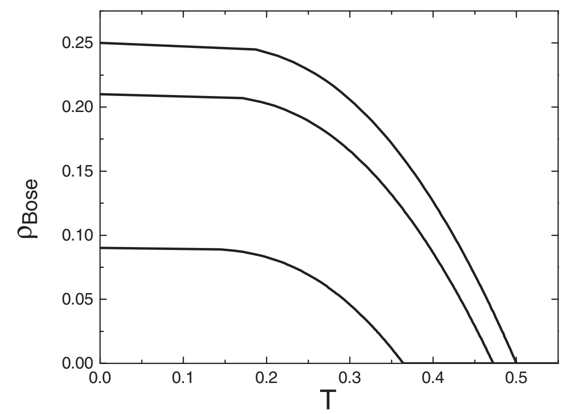

FIG. 4. The density of the Bose-Einstein condensate for the hardcore bosons versus temperature (dimensionless), for different $p=0.5$, 0.3, and 0.1 (from top to bottom).

$$\rho_n(\beta) = \frac{1}{Z}\sum_{r=0}^{N} e^{-\beta E_r}\mathrm{Tr}_{L-n}(\sigma_{L,N,r})$$

denotes the thermal RDM. For each given β the major contribution to the expression for $S_{(n)}(\beta)$ Eq. (50) comes from terms with given $r/L=\mu^*$ ratio, minimizing $\Lambda_{\min}$ in Eq. (47). For zero temperature $T=0$, the $S_{(n)}(\beta)$ is given by the expression Eq. (45). Above the critical temperature $T>T_c$ the $S_{(n)}(\beta)$ is given by Eq. (46). Note that the expression Eq. (46) coincides with the Gibbs entropy obtained from the spectrum of the whole system Eq. (3) in the thermodynamic limit $E(L,\mu,p)/L\approx\mu-\mu^2+p^2$, as

$$S_{Gibbs} = \frac{1}{L}\lim_{L\to\infty}\frac{\beta\langle E-F\rangle}{L}, \qquad (51)$$

where $F/L=\Lambda_{\min}/\beta$ and $\Lambda_{\min}$ is given by Eq. (47). Inserting the expressions for E and F into Eq. (51) we obtain Gibbs entropy

$$S_{Gibbs} = -\mu \log \mu - (1-\mu)\log(1-\mu).$$

For intermediate temperatures $0<T<T_c$, the entropy $S_{(n)}(\beta)$ is given in the thermodynamic limit by the general expression Eq. (42) which includes both the Gibbs contribution proportional to n and the quantum $T=0$ contribution proportional to $\log n$ [45].

Combining these results together we have [35]

$$S_{(n)} = \begin{cases} \frac{1}{2}\log n + \frac{1}{2}\log_2 2\pi e p q & \text{for } T=0, \\ S_{Gibbs} n + \frac{1}{2}\log n + R(p,\mu) & \text{for } 0<T<T_c, \\ S_{Gibbs} n & \text{for } T\geq T_c, \end{cases}$$

which clearly show the crossover from the pure quantum ($T=0$) regime to classical thermodynamics ($T\geq T_c$).

X. CONCLUSIONS

In this paper, we have presented a detailed investigation of the spectral properties of the RDM and of the VNE of permutational invariant quantum many-body systems for arbitrary parameters. To this regard we have used the irreducible representations of the symmetric group $\mathbf{S}_n$ and the conservation of the number of particles (S^z for the case of spins) to achieve the complete block diagonalization of the RDM for arbitrary initial states, sizes of the subsystem, symmetry properties and filling factors. An analytical expression for the RDM spectrum has been rigorously proved in the thermodynamical limit. Several sum rules and recurrence relations which are linked to symmetry properties and are satisfied by the RDM eigenvalues for arbitrary parameters, were considered. Particle-hole exchange and the half-filling symmetry were also discussed. The distribution function of RDM eigenvalues has been investigated in the thermodynamical limit for which we proved that it approaches a Gaussian as the size n of the block increases.

As a specific application we considered the case of a system of N hard-core bosons with infinite range interactions which undergo a Bose-Einstein condensation at $T=T_c$. For this system we investigated the thermal RDM and the VNE as a function of the block size and of the temperature, showing the existence of a crossover from (quantum) logarithmic behavior of the VNE at $T=0$ to a purely (classical) linear one for $T\geq T_c$.

The results of this paper show that, in spite of their infinite-range interactions, permutational invariant systems have very interesting and nontrivial RDM and VNE properties which allow to investigate the entanglement in the system from purely quantum behavior to classical thermodynamics. A challenging problem for the future will be to investigate implications of our results for RDM and VNE of many-body systems with finite range interactions, taking advantage of the fact that any finite symmetry group (like the cyclic group of translational invariant systems) is a subgroup of the permutation group.

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APPENDIX A: ONE STEP RDM REDUCTION EIGENVALUES

In this appendix we compute the eigenvalues involved in the one step RDM reduction of Sec. V The λ-s are determined by recursive application of the sum rules Eqs. (15) and (22) to sectors $k=s,s+1,\ldots,n-s$. Suppose we know all $\lambda^{n,k,s}_{n-1,k,s'}$ for a given sector k. Going from k to $k+1$, the sum rule Eq. (22) gives (apply the sum for case $L\to n, N\to k+1, r\to s, n\to n-1, k\to k, s\to s'$)

$$\lambda^{n,k,s}_{n-1,k,s'}+\lambda^{n,k+1,s}_{n-1,k,s'}=\frac{k-2s+1}{n-2s'}\frac{1}{\deg_{n,s}},\quad \text{for } s'=s,s-1, \tag{A1}$$

from which $\lambda^{n,k+1,s}_{n-1,k,s'}$ is determined. Similarly, from the sum rule Eq. (15) we can determine eigenvalues $\lambda^{n,k+1,s}_{n-1,k+1,s'}$ of the $k+1$ sector via

$$\lambda^{n,k,s}_{n-1,k,s'}+\lambda^{n,k,s}_{n-1,k-1,s'}=\frac{1}{\deg_{n,s}},\quad \text{for } s'=s,s-1. \tag{A2}$$

To start the recursive procedure the knowledge of $\lambda^{n,k,s}_{n-1,k,s}$ in the sector $k=s$ is required. These are easily obtained by observing that Eq. (23) for the sector $k=s$ involves only three contributions, e.g.,

$$\mathrm{Tr}_1 \varsigma_{n,k=s,s}=\lambda^{n,s,s}_{n-1,s,s}\sigma_{n-1,s,s}+\lambda^{n,s,s}_{n-1,s,s-1}\sigma_{n-1,s,s-1}+\lambda^{n,s,s}_{n-1,s-1,s-1}\sigma_{n-1,s-1,s-1}.$$

because a filled YT of type $\{n-s-1,s\}_{(k=s-1)}$ cannot exist. Then, the identity Eq. (A2) applied for $s'=s$ gives $\lambda^{n,s,s}_{n-1,s,s}=\frac{1}{\deg_{n,s}}$, while the identity Eq. (A1) applied for $k=s-1$ and $s'=s-1$ gives $\lambda^{n,s,s}_{n-1,s-1,s-1}=\frac{n-2s+1}{n-2s+2}\frac{1}{\deg_{n,s}}$. Finally, since the sum of all eigenvalues in the sector is 1, we obtain the remaining term as $\lambda^{n,s,s}_{n-1,s,s-1}\deg_{n-1,s-1}=1-\deg_{n-1,s}\lambda^{n,s,s}_{n-1,s,s}-\deg_{n-1,s-1}\lambda^{n,s,s}_{n-1,s-1,s-1}=\frac{1}{n-2s+2}\frac{\deg_{n-1,s-1}}{\deg_{n,s}}$ (notice that the normalization of the eigenvalues follows from the identity $\deg_{n,s}=\deg_{n-1,s}+\deg_{n-1,s-1}$). Alternatively, the unknown coefficient $\lambda^{n,s,s}_{n-1,s,s-1}$ can also be determined using the Eq. (A2) for $s'=s-1$. Having determined the λ-s of the sector $k=s$ one can determine the ones of sector $k=s+1$ etc. Iterating the procedure, leads to the final expressions in Eq. (25).

APPENDIX B: LIMITING CASES OF RDM EIGENVALUES

Different limiting cases of Eq. (28) are computed below.

(i) Case $r=0$. From Eq. (28) we see that the sums on m and on j contribute only with the terms $m=0$ and $j=0$ and eigenvalues reduce to

$$\lambda^{L,N,0}_{n,k,0}=\frac{\binom{L-n}{N-k}}{\binom{L}{N}}\sum_{i=0}^{k}\binom{k}{i}\binom{n-k}{i}=\frac{\binom{L-n}{N-k}}{\binom{L}{N}}\binom{n}{k}.$$

This is the same expression obtained for symmetric states in [12].

(ii) Case $k=s=n/2$ (n even). The sum on i in Eq. (28) contributes only with $i=0$ and $\lambda^{L,N,r}_{n,n/2,n/2}$ reduces to

$$\frac{\binom{L-n}{N-n/2}}{\binom{L}{N}}\sum_{j=0}^{k}\frac{(-1)^j\binom{\frac{n}{2}}{j}}{\binom{L-N}{j}\binom{N}{j}}\times\sum_{m=0}^{j}(-1)^m\binom{L-N-r}{j-m}\binom{N-r}{j-m}\binom{r}{m}.$$

The double sum in this expression is evaluated as $\frac{\binom{L}{N}}{\binom{L-n}{N-n/2}}\frac{\binom{L-n}{r-n/2}-\binom{L-n}{r-n/2-1}}{\binom{L}{r}-\binom{L}{r-1}}$ and the result in Eq. (16) is obtained.

(iii) Case $L\to\infty$. In this case there is only the term $m=0$ which contributes to the m sum in Eq. (28) (other terms will vanish in the limit) so that $\lim_{L\to\infty}\lambda_{n,k,s}^{L,N,r}$ becomes:

$$\frac{\binom{L-n}{N-k}}{\binom{L}{N}}\sum_{i=0}^{k-s}\binom{k-s}{i}\binom{n-k-s}{i}$$

$$\times\sum_{j=0}^{k-i}(-1)^j\binom{s}{j}\frac{\binom{L-N-r}{j+i}\binom{N-r}{j+i}}{\binom{L-N}{j+i}\binom{N}{j+i}}$$

$$\approx p^kq^{n-k}\sum_{i=0}^{k-s}\binom{k-s}{i}\binom{n-k-s}{i}(-1)^i\sum_{j=i}^{k}(-1)^j\binom{s}{j-i}\eta^j, \tag{B1}$$

where we used

$$\frac{\binom{L-n}{N-k}}{\binom{L}{N}}\approx p^kq^{n-k},\quad \frac{\binom{L-N-r}{j}\binom{N-r}{j}}{\binom{L-N}{j}\binom{N}{j}}\approx\eta^j,$$

with p,η given by Eqs. (29) and (32), respectively, and with $q=1-p$. The last summation in Eq. (B1) can be explicitly carried out as

$$\sum_{j=i}^{k}(-1)^j\eta^j\binom{s}{j-i}=\sum_{u=0}^{k-i}(-\eta)^{u+i}\binom{s}{u}=(-\eta)^i(1-\eta)^s.$$

for any $0\le i\le k-s$. Substitution into Eq. (B1) gives

$$\lim_{L\to\infty}\lambda_{n,k,s}^{L,N,r}=p^kq^{n-k}(1-\eta)^s\sum_{i=0}^{k-s}\eta^i\binom{k-s}{i}\binom{n-k-s}{i},$$

this proving Eq. (30).

APPENDIX C: MAXIMUM OF $Q(k,s)$

In this appendix we prove that the maximum of $Q(k,s)$, $Q_{\max}$, occurs at the point ($k_{\max}=nq$, $s_{\max}=n\mu$), assuming $n\gg1$ and neglecting all finite size corrections of order $O(\frac{1}{n})$. To this regard we use the thermodynamic expression of Q given in Eq. (38) and the following identities

$$\frac{\partial}{\partial i}\log\binom{M}{i}\approx\log\frac{M-i}{i},\quad \frac{\partial}{\partial k}\log\binom{M}{i}\approx M'\log\frac{M}{M-i}, \tag{C1}$$

which directly follow from the Stirling formula. Observing that $\frac{\partial}{\partial k}F=F\frac{\partial}{\partial k}(\log F)$, we have can compute the derivative with respect to k as

$$\frac{\partial Q}{\partial k}\equiv Q'$$

$$=Q\frac{\partial}{\partial k}\log[P]+P\sum_{i=0}^{k-s}\eta^i\binom{M}{i}\binom{K}{i}\frac{\partial}{\partial k}\log\left[\binom{M}{i}\binom{K}{i}\right]$$

$$\approx Q\log\frac{q}{p}+P\sum_{i=0}^{k-s}\eta^i\binom{M}{i}\binom{K}{i}$$

$$\times\left(M'\log\frac{M}{M-i}+K'\log\frac{K}{K-i}\right)$$

$$\approx Q\left(\log\frac{q}{p}+\log\frac{M}{M-i_{\max}}-\log\frac{K}{K-i_{\max}}\right), \tag{C2}$$

with the prime denoting derivation with respect to k. In the last passage we used $M'=\frac{\partial}{\partial k}(k-s)=1$, $K'=-1$ and the fact that the logarithm is a slowly varying function to approximate the log terms in the sum with their values taken at the point $i=i_{\max}$ for which

$$\frac{\partial}{\partial i}\log\left[\eta^i\binom{M}{i}\binom{K}{i}\right]=0.$$

From this, using Eq. (C1), it follows that

$$i_{\max}^2(-1+\eta)-\eta(M+K)i_{\max}+\eta MK=0, \tag{C3}$$

which gives, using Eq. (32),

$$i_{\max}=\eta\frac{npq}{1-\mu}=n\frac{(p-\mu)(q-\mu)}{1-\mu}. \tag{C4}$$

It is convenient to introduce $i_{\max}=M_0\alpha=K_0\gamma$ where the subscript zero denotes (here and below) the evaluation at the point ($k_{\max}=nq$, $s_{\max}=n\mu$), e.g., $M_0=n(q-\mu)$, $K_0=n(1-q-\mu)=n(p-\mu)$. We then have

$$\left(\frac{M}{M-i_{\max}}\right)_0=\frac{1}{\beta},\quad \left(\frac{K}{K-i_{\max}}\right)_0=\frac{1}{\delta},$$

with quantities α, $\beta=1-\alpha$, γ, and $\delta=1-\gamma$ given by

$$\alpha=\frac{p-\mu}{1-\mu},\quad \beta=\frac{q}{1-\mu},\quad \gamma=\frac{q-\mu}{1-\mu},\quad \delta=\frac{p}{1-\mu}. \tag{C5}$$

Thus, from Eq. (C2) we obtain

$$\left(\frac{\partial Q}{\partial k}\right)_0=Q_0\left(\log\frac{q}{p}+\log\frac{\delta}{\beta}\right)=0,$$

where $Q_0=Q(k=k_{\max},s=s_{\max})\equiv Q_{\max}$. Similarly, we find that

$$\frac{\partial Q}{\partial s}=Q\left[\log\frac{n-s}{s}+\log(1-\eta)+O\left(\frac{1}{n}\right)\right.$$

$$\left.-\log\frac{M}{M-i_{\max}}-\log\frac{K}{K-i_{\max}}\right],$$

with the term $O(\frac{1}{n})$ arising from the differentiation of the constant $\frac{n-2s+1}{n-s+1}$, and where we have again used the slowness of log function and $\frac{\partial M}{\partial s}=\frac{\partial K}{\partial s}=-1$. At the point $k_{\max}=nq$, $s_{\max}=n\mu$ we have

$$\left(\frac{\partial Q}{\partial s}\right)_0 \approx Q_0\left[\log\frac{1-\mu}{\mu}+\log\frac{\mu(1-\mu)}{pq}+\log(\beta\delta)\right]=0.$$

Having proved that $k=nq$, $s=n\mu$ is an extremal point for $Q(k,s)$, we check the positiveness of the quadratic form $\Theta \equiv -(\frac{\partial^2 Q}{\partial k^2}\delta k^2+2\frac{\partial^2 Q}{\partial k \partial s}\delta k\,\delta s+\frac{\partial^2 Q}{\partial s^2}\delta s^2)$ at this point. We have

$$\left(\frac{\partial^2 Q}{\partial k^2}\right)_0 = Q_0\frac{\partial}{\partial k}\left(\log\frac{q}{p}+\log\frac{M}{M-i_{\max}}-\log\frac{K}{K-i_{\max}}\right) = \frac{M'}{M}-\frac{(M-i_{\max})'}{M-i_{\max}}-\frac{K'}{K}+\frac{(K-i_{\max})'}{K-i_{\max}}.$$

By differentiating Eq. (C3) with respect to k and to s and using Eq. (C4), we obtain

$$\left(\frac{\partial i_{\max}}{\partial k}\right)_0 = p-q, \quad \left(\frac{\partial i_{\max}}{\partial s}\right)_0 = -1+\frac{2pq}{1-\mu},$$

which are needed for the second derivatives of Q. We find:

$$\frac{1}{Q_0}\left(\frac{\partial^2 Q}{\partial k\,\partial s}\right)_0 = \frac{1}{Q_0}\left(\frac{\partial^2 Q}{\partial s\,\partial k}\right)_0 = \frac{(1-2\mu)(p-q)}{n(p-\mu)(q-\mu)} \equiv -\frac{1}{B},$$

$$\frac{1}{Q_0}\left(\frac{\partial^2 Q}{\partial s^2}\right)_0 = -\frac{1}{n\mu(1-\mu)}-\frac{(p-q)^2}{n(p-\mu)(q-\mu)} \equiv -\frac{1}{C},$$

$$\frac{1}{Q_0}\left(\frac{\partial^2 Q}{\partial k^2}\right)_0 = -\frac{(1-2\mu)^2}{n(p-\mu)(q-\mu)} \equiv -\frac{1}{D}, \qquad \text{(C6)}$$

which coincide with the expressions given in Eq. (37). Moreover, we see that $C>0, D>0, CD-B^2>0$, this implying that the above quadratic form Θ is positive definite and $(k=nq,\ s=n\mu)$ is a maximum.

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[45] Strictly speaking, Eq. (42) gives the VNE microcanonical entropy corresponding to a macrostate with the energy $E(\mu^*)$ related to β by Eq. (48). The VNE computed in the canonical ensemble Eq. (50) is expected to have the same leading (linear in n) and subleading (logarithmic in n) contributions.