An analytical probabilistic approach to the ground state of lattice quantum systems: exact results in terms of a cumulant expansion

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Abstract. We present a large deviation analysis of a recently proposed probabilistic approach to the study of the ground-state properties of lattice quantum systems. The ground-state energy as well as the correlation functions in the ground state are exactly determined as series expansions in the cumulants of the multiplicities of the potential and hopping energies assumed by the system during its long-time evolution. Once these cumulants are known, even at a finite order, our approach provides the ground state analytically as a function of the Hamiltonian parameters. A scenario of possible applications of the analytic character of the present approach is discussed.

Keywords: correlation functions, rigorous results in statistical mechanics, other numerical approaches, series expansions

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Contents

1. Introduction

The real- or imaginary-time dynamics of systems described by a finite Hamiltonian matrix, representing bosonic or fermionic degrees of freedom, admits an exact probabilistic representation in terms of a proper collection of independent Poisson processes [1]–[3]. For a lattice system, the Poisson processes are associated with the links of the lattice and the probabilistic representation leads to an optimal algorithm [3] which coincides with the Green function quantum Monte Carlo method in the limit when the latter becomes exact [4].

Recently, in [5] we have exploited the above probabilistic representation to derive analytical estimations for the matrix elements of the evolution operator in the long-time limit. In this way, approximations for the ground-state energy, as well as for the expectation of a generic operator in the ground state of a lattice system without a sign problem, have been obtained as the solution of a simple scalar equation. The results presented in [5] were based on the application of a central limit theorem to the rescaled multiplicities of the values assumed by the potential and hopping energies in the configurations dynamically visited by the system (see also [6] for details on the corresponding probability density).

The approximated scalar equation for the ground-state energy obtained by using the central limit theorem contains only the first two statistical moments of the multiplicities mentioned above and, as anticipated in [5], suggests that it is a second-order truncation of an exact cumulant expansion. In this paper, after reviewing in detail the approach developed in [5], we perform a large deviation analysis of the relevant probability density and obtain this exact cumulant expansion. In principle, if all the cumulants are known, we provide a scalar equation whose straightforward solution is the exact ground-state

energy of the system. In practice, we measure the cumulants via a statistical sampling and only a finite number of them are available. The corresponding truncated equation provides ground-state energies whose level of approximation depends on the values of the Hamiltonian parameters and on the size of the system. However, the convergence as a function of the number of cumulants is rather fast and, as shown in some example cases, the use of the first few cumulants provides results indistinguishable from those obtained from exact numerical simulations.

The spirit of our approach is different from that of Monte Carlo simulations. In the latter case, the accumulated statistical data provide information on the specific system under investigation and new simulations must be performed each time the value of a single parameter of the model is changed. On the other hand, our approach is semi-analytical in the sense that we have an exact expression for the ground-state energy, in which some statistical data, namely the cumulants of the multiplicities mentioned above, must be provided as an input. However, these multiplicities, and so the corresponding cumulants, do not depend on the values of the parameters of the model, only on the structure of the Hamiltonian operator (form of the hopping and interaction terms, size of the system and so on). For instance, in the case of N spin-up and N spin-down particles with on-site interaction of strength γ the multiplicities depend on the spectrum of the possible on-site pairs, $0, 1, 2, \ldots, N$, not on γ which represents, therefore, a parameter with respect to which we have analytical results. The analyticity with respect to the parameters of the Hamiltonian allows the determination of the expectation of a generic operator in the ground state of the system via the Hellmann–Feynman theorem and suggests other potential applications that we will discuss at the end.

The paper is organized as follows. In section 2 we briefly review the probabilistic representation of quantum dynamics for generic lattice systems. In this way, the ground-state energy is obtained as the expectation of a suitable stochastic functional. In section 3 we summarize our main result, namely an exact formula for the ground-state energy, and provide an outline of its proof. In the four subsections of the core section 4, we develop in full detail this proof via the analytical determination, in the limit of an infinitely long time, of the expectation of the stochastic functional providing the ground-state energy. In section 4.1, we decompose the expectation in a series of canonical averages of weights, which are calculated in section 4.2. The canonical averages are evaluated via a cumulant expansion theorem in section 4.3 and are finally resummed in section 4.4, where the exact scalar equation for the ground-state energy is presented. In section 5 we discuss the numerical evaluation of the cumulants which appear in our formula for the ground-state energy. In the same section, we also study some example cases and compare the results from using our formula with those from exact numerical calculations. Finally, general features of our approach and future applications are summarized and discussed in section 6.

Up to section 4.2, we carry on the development both for hard-core bosons and fermions, whereas subsequently we limit the method to hard-core bosons, postponing consideration of the fermion case to a later work.

2. Exact probabilistic representation of lattice dynamics

In this section we review the exact probabilistic representation of the imaginary- or real-time dynamics of a system of bosons or fermions on a lattice; see [3] for a detailed

description. This representation is the basis of our approach to studying the ground-state properties of the system in a semi-analytical way [5]. We concentrate on a simple exclusion dynamics, in which multiple occupancies of the lattice sites are forbidden, i.e. fermions or hard-core bosons are considered.

Let Λ be any finite lattice with cardinality $|\Lambda|$ and $1, 2, \ldots, |\Lambda|$ be some total ordering of the lattice sites. The dynamics of a system of hard-core bosons or fermions on this lattice is effectively described in terms of commuting or anticommuting destruction operators $\hat{c}_{i\sigma}$ with the property $(\hat{c}_{i\sigma})^2 = 0$. Here, $i = 1, 2, \ldots, |\Lambda|$ is the site index and $\sigma = \uparrow\downarrow$ the spin, or an arbitrary internal index. The system can be represented in terms of Fock states, $\boldsymbol{n} \in \mathbb{F}$, $\boldsymbol{n} = (n_{1\uparrow}, n_{1\downarrow}, \ldots, n_{|\Lambda|\uparrow}, n_{|\Lambda|\downarrow})$, where $n_{i\sigma}$ is the lattice occupation number of the site i with spin σ taking the value 0 or 1. The number of Fock states is

$$|\mathbb{F}| = \binom{|\Lambda|}{N_\uparrow}\binom{|\Lambda|}{N_\downarrow}, \tag{1}$$

where N_σ is the number of particles with spin σ.

We assume the system to be described by the Hamiltonian

$$\hat{H} = \hat{K} + \hat{V}, \tag{2}$$

where $\hat{K}$ and $\hat{V}$ are the kinetic and potential operators, respectively. The potential operator $\hat{V}$ is arbitrary, e.g. for the Hubbard model $\hat{V} = \sum_{i\in\Lambda} \gamma_i \hat{c}_{i\uparrow}^\dagger \hat{c}_{i\uparrow} \hat{c}_{i\downarrow}^\dagger \hat{c}_{i\downarrow}$. For the kinetic operator we assume the quadratic form

$$\hat{K} = -\sum_{i\neq j\in\Lambda} \sum_{\sigma=\uparrow\downarrow} \eta_{ij\sigma} \mathrm{e}^{\mathrm{i}\theta_{ij\sigma}} \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma}, \tag{3}$$

with $\eta_{ij\sigma}, \theta_{ij\sigma} \in \mathbb{R}$ and $\eta_{ij\sigma} \geq 0$. The case $\theta_{ij\sigma} \neq 0$ is obtained in the presence of a magnetic field. In principle, our approach can be extended to more general kinetic operators. The essential feature to be noted is that in the Fock representation $\hat{V}$ is diagonal whereas $\hat{K}$ is off-diagonal.

In order to study the ground-state properties of the Hamiltonian $\hat{H}$, it is sufficient to evaluate the long-time behaviour of $\sum_{\boldsymbol{n}} \langle \boldsymbol{n} | \mathrm{e}^{-\hat{H}t} | \boldsymbol{n}_0 \rangle$. In fact, the ground-state energy is given by

$$E_0 = \lim_{t\to\infty} -\partial_t \log \sum_{\boldsymbol{n}} \langle \boldsymbol{n} | \mathrm{e}^{-\hat{H}t} | \boldsymbol{n}_0 \rangle. \tag{4}$$

The quantum expectation of a generic operator $\hat{O}$ in the ground state of $\hat{H}$ can be obtained by evaluating the ground-state energy $E_0(\xi)$ of the modified Hamiltonian $\hat{H} + \xi\hat{O}$ and using the Hellmann–Feynman identity

$$\frac{\langle E_0(\xi) | \partial_\xi \hat{H}(\xi) | E_0(\xi) \rangle}{\langle E_0(\xi) | E_0(\xi) \rangle} = \partial_\xi E_0(\xi). \tag{5}$$

Let Γ_σ be the set of system links with spin σ, i.e. the pairs (i, j) with $i \neq j$ and $i, j \in \Lambda$ such that $\eta_{ij\sigma} \neq 0$. With each link (i, j) with spin σ we associate the value

$$\lambda_{ij\sigma}(\boldsymbol{n}) = \langle \boldsymbol{n} \oplus \mathbf{1}_{i\sigma} \oplus \mathbf{1}_{j\sigma} | \mathrm{e}^{\mathrm{i}\theta_{ij\sigma}} \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + \mathrm{e}^{\mathrm{i}\theta_{ji\sigma}} \hat{c}_{j\sigma}^\dagger \hat{c}_{i\sigma} | \boldsymbol{n} \rangle, \tag{6}$$

where $\mathbf{1}_{i\sigma} = (0, \ldots, 0, 1_{i\sigma}, 0, \ldots, 0)$ and $n \oplus n' = (n + n') \mathrm{mod} 2$. We may have $|\lambda_{ij\sigma}| = 0, 1$ only. A link (i, j) with spin σ is called active if $\lambda_{ij\sigma} \neq 0$. For $\theta_{ij\sigma} \equiv 0$, in the case of

hard-core bosons an active link can take only the positive value $\lambda_{ij\sigma} = 1$, whereas in the case of fermions an active link is either 1 or -1, depending on whether the number of particles present between the sites i and j, $\sum_{k=i+1}^{j-1} n_{k\sigma}$, is even or odd.

Let $\{N_{ij\sigma}^t\}$ be a family of $|\Gamma| = |\Gamma_\uparrow \cup \Gamma_\downarrow|$ independent Poisson process with jump rate ρ. These processes are in a one-to-one correspondence with the links of the lattice. At each jump of a Poisson process relating sites i and j with spin σ and taking place at a given configuration $\boldsymbol{n}$, a particle of spin σ moves from site i to site j or vice versa if $|\lambda_{ij\sigma}(\boldsymbol{n})| = 1$, whereas the lattice configuration $\boldsymbol{n}$ remains unchanged if $\lambda_{ij\sigma}(\boldsymbol{n}) = 0$. By arranging the jumps according to the times s_k, $k = 1, \ldots, N_t$, at which they take place in the interval $[0, t)$, we define a trajectory as the sequence of configurations $\boldsymbol{n}_1, \boldsymbol{n}_2, \ldots, \boldsymbol{n}_{N_t}$ generated from a chosen initial configuration $\boldsymbol{n}_0$ by exchanging, at each jump of the Poisson process $N_{ij\sigma}^t$, the occupations of the sites $n_{i\sigma}$ and $n_{j\sigma}$. The number of jumps N_t is, of course, a random integer associated with each trajectory. Let (i_k, j_k) with spin σ_k be the link jumping at the time s_k. By putting for brevity

$$\lambda_k = \lambda_{i_k j_k \sigma_k}(\boldsymbol{n}_{k-1}), \tag{7}$$

$$\eta_k = \eta_{i_k j_k \sigma_k}, \tag{8}$$

we define with $\lambda_1, \lambda_2, \ldots, \lambda_{N_t}$, and $\eta_1, \eta_2, \ldots, \eta_{N_t}$, the sequences of the corresponding link values and hopping parameters. With each trajectory, we also associate the sequences $A_0, A_1, \ldots, A_{N_t}$ and $V_0, V_1 \ldots, V_{N_t}$, representing the number of active links and the potential energy of the configurations visited:

$$A_k = \sum_{\sigma=\uparrow\downarrow} \sum_{(i,j)\in\Gamma_\sigma} |\lambda_{ij\sigma}(\boldsymbol{n}_k)| \tag{9}$$

$$V_k = \langle \boldsymbol{n}_k | \hat{V} | \boldsymbol{n}_k \rangle. \tag{10}$$

For later use, we also define

$$T_k = A_k \eta_{k+1}/\epsilon, \tag{11}$$

where ϵ is an arbitrary reference energy.

At any finite time t, the following exact probabilistic representation holds [3]:

$$\langle \boldsymbol{n} | \mathrm{e}^{-Ht} | \boldsymbol{n}_0 \rangle = \mathsf{E}(\delta_{\boldsymbol{n},\boldsymbol{n}_{N_t}} \mathcal{M}_{\boldsymbol{n}_0}^t), \tag{12}$$

where the stochastic functional $\mathcal{M}_{\boldsymbol{n}_0}^t$ is defined as

$$\mathcal{M}_{\boldsymbol{n}_0}^t = \mathrm{e}^{|\Gamma|\rho t}\left(\prod_{k=1}^{N_t} \frac{\eta_k}{\rho} \lambda_k \mathrm{e}^{-V_{k-1}(s_k - s_{k-1})}\right) \mathrm{e}^{-V_{N_t}(t - s_{N_t})} \tag{13}$$

if $N_t > 0$ and $\mathcal{M}_{\boldsymbol{n}_0}^t = \mathrm{e}^{|\Gamma|\rho t} \mathrm{e}^{-V_0 t}$ if $N_t = 0$ and the symbol $\mathsf{E}(\cdot)$ means the expectation over the $|\Gamma|$ independent Poisson processes. In equation (13), we put $s_0 = 0$. According to this representation, we have

$$\sum_{\boldsymbol{n}} \langle \boldsymbol{n} | \mathrm{e}^{-Ht} | \boldsymbol{n}_0 \rangle = \mathsf{E}(\mathcal{M}_{\boldsymbol{n}_0}^t), \tag{14}$$

so that we can evaluate the ground-state energy as

$$E_0 = \lim_{t\to\infty} -\partial_t \log \mathsf{E}(\mathcal{M}_{\boldsymbol{n}_0}^t). \tag{15}$$

In the following, we will be able to reduce the study of the expectation of the stochastic functional (13) to the study of simpler canonical averages over the stochastic trajectories $\boldsymbol{n}_0, \boldsymbol{n}_1, \boldsymbol{n}_2, \ldots$ in which $\boldsymbol{n}_k \neq \boldsymbol{n}_{k-1}$ for any $k > 1$, i.e. trajectories in which only jumps corresponding to active links are considered, and the jumping times are disregarded (integrated out). These sequences of configurations $\boldsymbol{n}_0, \boldsymbol{n}_1, \boldsymbol{n}_2, \ldots$ constitute a homogeneous Markov chain in a finite state space, $\mathbb{F}$, with the transition matrix $\boldsymbol{P}$ defined by

$$
P_{\boldsymbol{n}, \boldsymbol{n}'} = \begin{cases} A(\boldsymbol{n})^{-1} & \text{if } \exists\ \sigma \in \{\uparrow, \downarrow\} \text{ and } (i,j) \in \Gamma_\sigma: \\ & \qquad \boldsymbol{n}' = \boldsymbol{n} \oplus \mathbf{1}_{i\sigma} \oplus \mathbf{1}_{j\sigma} \text{ and } \lambda_{ij\sigma}(\boldsymbol{n}) \neq 0 \\ 0 & \text{otherwise,} \end{cases} \tag{16}
$$

where $A(\boldsymbol{n}) = \sum_{\sigma=\uparrow\downarrow} \sum_{(i,j) \in \Gamma_\sigma} |\lambda_{ij\sigma}(\boldsymbol{n})|$ is the number of active links of the configuration $\boldsymbol{n}$. Note that $\sum_{\boldsymbol{n}'} P_{\boldsymbol{n}, \boldsymbol{n}'} = 1$ according to the fact that $P_{\boldsymbol{n}, \boldsymbol{n}'}$ is the probability for the transition $\boldsymbol{n} \to \boldsymbol{n}'$. Finally, the canonical averages mentioned above are introduced for trajectories with a finite number of jumps in the following way. Given an initial state $\boldsymbol{n}_0$ and an application $f : \mathbb{F}^{N+1} \to \mathbb{C}$, a function of $\boldsymbol{n}_0$ and of the consecutive N configurations $\boldsymbol{n}_1, \boldsymbol{n}_2 \ldots, \boldsymbol{n}_N$, we will indicate as $\langle f \rangle_N$, called the canonical average, the average of f sampled with respect to the measure induced by the transition probability (16) iterated N times. Similarly, we can consider canonical averages in which the initial state is not a single Fock state, $\boldsymbol{n}_0$, but an ensemble with distribution $\boldsymbol{\pi}_0$. An ensemble of particular interest is the invariant measure $\boldsymbol{\pi}$, defined as the left eigenvector of the transition matrix, $\boldsymbol{\pi}^{\mathrm{T}} \boldsymbol{P} = \boldsymbol{\pi}^{\mathrm{T}}$. It is simple to verify that

$$
\pi(\boldsymbol{n}) = \frac{A(\boldsymbol{n})}{\sum_{\boldsymbol{n}'} A(\boldsymbol{n}')}. \tag{17}
$$

3. Main result and outline of the proof

Evaluating the expectation $\mathsf{E}(\mathcal{M}_{\boldsymbol{n}_0}^t)$ over the detailed realizations of the stochastic processes specified above can be done numerically by a Monte Carlo method [3]. The efficiency of the corresponding numerical algorithm is discussed in detail in [7]. In this paper, we are interested in obtaining analytical expressions of $\mathsf{E}(\mathcal{M}_{\boldsymbol{n}_0}^t)$, which are asymptotically exact in the limit $t \to \infty$, and providing an exact formula for the ground-state energy by using equation (15).

Let us call $\mathscr{L}$, $\mathscr{V}$ and $\mathscr{T}$ the sets of all the possible different values λ, V and T assumed by equations (7), (10) and (11), respectively, along a trajectory $\boldsymbol{n}_0, \boldsymbol{n}_1, \boldsymbol{n}_2, \ldots$ formed by infinitely many jumps. Let $m_{\mathscr{L}}$, $m_{\mathscr{V}}$ and $m_{\mathscr{T}}$ be the corresponding cardinalities. Since any configuration can be obtained from any other one by a finite number of jumps, i.e. the Markov chain of the trajectories is irreducible, the elements in the sets $\mathscr{L}$, $\mathscr{V}$ and $\mathscr{T}$ do not depend on the initial configuration $\boldsymbol{n}_0$. Moreover, the value of their elements and, in particular, their number depend only on the structure of the Hamiltonian operator, not on the values of the Hamiltonian parameters.

As we shall show, a crucial point is that, if we consider the conditional expectation in which the number of jumps N is fixed, $\mathsf{E}(\mathcal{M}_{\boldsymbol{n}_0}^t | N_t = N)$, and integrate over all the possible jump times, what matters in determining the value of $\mathsf{E}(\mathcal{M}_{\boldsymbol{n}_0}^t | N_t = N)$ is not the

detailed sequences of the configurations visited but just the multiplicities, or numbers of occurrences, N_λ, N_V and N_T of the variables λ, V and T, respectively. Explicitly, for a trajectory with N jumps, these multiplicities are defined as

$$N_\lambda = \sum_{k=0}^{N-1} \delta_{\lambda_k, \lambda}, \tag{18a}$$

$$N_V = \sum_{k=0}^{N} \delta_{V_k, V}, \tag{18b}$$

$$N_T = \sum_{k=0}^{N-1} \delta_{T_k, T}, \tag{18c}$$

with λ_k, V_k and T_k given by equations (7), (10) and (11). The expectation $\mathsf{E}(\mathcal{M}_{\boldsymbol{n}_0}^t | N_t = N)$ is thus reduced to an average over the variables N_λ, N_V and N_T. In other words, after the stochastic times have been integrated out, the knowledge of all the canonical moments

$$\langle N_{\alpha_1} \cdots N_{\alpha_k} \rangle_N, \tag{19}$$

where $\alpha_i \in \mathscr{H} = \mathscr{V} \cup \mathscr{T} \cup \mathscr{L}$, $i = 1, \ldots, k$, determines completely the expectation $\mathsf{E}(\mathcal{M}_{\boldsymbol{n}_0}^t | N_t = N)$.

Let us consider the case of hard-core bosons in the absence of magnetic fields, i.e. the case for which $\mathscr{L} = \{1\}$. As we will prove, after the integration of the stochastic times, the conditional expectation $\mathsf{E}(\mathcal{M}_{\boldsymbol{n}_0}^t | N_t = N)$ becomes

$$\mathsf{E}\left(\mathcal{M}_{\boldsymbol{n}_0}^t | N_t = N\right) = \left\langle \mathcal{W}_N(t) \prod_{T \in \mathscr{T}} T^{N_T} \right\rangle_N, \tag{20}$$

where $\mathcal{W}_N(t)$, called the weight, is a function that depends only on the multiplicities of the potential (18b), whereas the other factor is a purely kinetic function that depends only on the multiplicities (18c).

In order to understand the behaviour of equation (20), and then of equation (14), let us start by considering a non-interacting system with $\hat{V} \equiv 0$. In this case we have $\mathscr{V} = \{0\}$ and the weights have the simple exact expression $\mathcal{W}_N^{(0)}(t) = \epsilon^N t^N / N!$. Therefore for $\mathsf{E}(\mathcal{M}_{\boldsymbol{n}_0}^t | N_t = N)$ we are left with a residual canonical average over the variables N_T and we get

$$\mathsf{E}(\mathcal{M}_{\boldsymbol{n}_0}^t | N_t = N) = \frac{(\epsilon t)^N}{N!} \left\langle e^{\sum_T \log(T) N_T} \right\rangle_N \sim \frac{(a\epsilon t)^N}{N!}, \tag{21}$$

where a is a suitable value coming from the integration over N_T.

The result in equation (21) can be immediately obtained from the rough estimate $\langle \exp[\sum_T \log(T) N_T] \rangle_N \sim \text{const}^N$, based on the bounds $\exp[N \log(T_{\min})] \leq \langle \exp[\sum_T \log(T) N_T] \rangle_N \leq \exp[N \log(T_{\max})]$, which in turn follow from the normalization $\sum_{T \in \mathscr{T}} N_T = N$. By using a cumulant expansion theorem [8], however, it can be shown that this result becomes exact for $N \to \infty$ if we assume the existence of the following rescaled cumulants of the variables N_T:

$$\Sigma_{T_1, \ldots, T_k}^{(k)} = \lim_{N \to \infty} \frac{1}{N} \langle N_{T_1} \cdots N_{T_k} \rangle_N^{(c)}, \tag{22}$$

where by $\langle \cdot \rangle_N^{(c)}$ we indicate the cumulants, or connected correlation functions, sampled with respect to the measure induced by the transition matrix (16). The connection between these cumulants and the statistical moments introduced above is well known. For $k = 1$ we have $\langle N_{T_1} \rangle_N^{(c)} = \langle N_{T_1} \rangle_N$, for $k = 2$ $\langle N_{T_1} N_{T_2} \rangle_N^{(c)} = \langle N_{T_1} N_{T_2} \rangle_N - \langle N_{T_1} \rangle_N \langle N_{T_2} \rangle_N$ and so on.

Since the Markov chain with the transition matrix (16) is finite and irreducible, for $k = 1$ the existence of the limit (22) is ensured by an ergodic theorem [9]. On the other hand, for $k > 1$, the existence and the finiteness of the rescaled cumulants (22), or of the more general limits (26), follows from the exponential decay of the correlations of local functions of the configurations along the Markov chain. For the T variables, this property amounts to saying that for any k there exist positive constants b_k and $N_c(k)$ such that for any N,

$$|\langle \chi_{T_1}(\boldsymbol{n}_{h_1}) \cdots \chi_{T_k}(\boldsymbol{n}_{h_k}) \rangle_N^{(c)}| \leq b_k \exp\left(-\frac{h_{\max} - h_{\min}}{N_c(k)} \right), \tag{23}$$

where $\chi_T(\boldsymbol{n}) = \delta_{T(\boldsymbol{n}),T}$ is the characteristic function of the states T and $h_{\max}$ and $h_{\min}$ are the maximum and the minimum of the indices $0 \leq h_l \leq N$, $l = 1, \ldots, k$ along the chain. A numerical check of equation (23) for $k = 2$ will be shown in section 5.

Since the rightmost expression in equation (21) has, as a function of N, an exponentially leading maximum at $N = \epsilon a t$, we see that for t large an important consequence follows. The full expectation $\mathsf{E}(\mathcal{M}_{\boldsymbol{n}_0}^t) = \sum_{N=0}^{\infty} \mathsf{E}(\mathcal{M}_{\boldsymbol{n}_0}^t | N_t = N)$ takes exponentially leading contributions from terms with $N \sim \epsilon a t$. Therefore, for $t \to \infty$ we have that (i) the saddle point technique used to evaluate the canonical averages over N_T becomes exact and (ii) a further saddle point integration can be used to exactly resum the full expectation $\mathsf{E}(\mathcal{M}_{\boldsymbol{n}_0}^t)$. In conclusion, we obtain an exact expression for the ground-state energy, namely $\lim_{t\to\infty} -\partial_t \log \mathsf{E}(\mathcal{M}_{\boldsymbol{n}_0}^t)$.

For $\hat{V} \neq 0$, the above-described scenario remains essentially unchanged. In fact, even though in this case the integration of the stochastic times cannot be done exactly, it can be performed using a saddle point approximation, which becomes asymptotically exact for $N \to \infty$. Independently of their exact value, as we will prove later, the weights are bounded by $\mathcal{W}_N^{(0)}(t) \mathrm{e}^{-V_{\max} t} \leq \mathcal{W}_N(t) \leq \mathcal{W}_N^{(0)}(t) \mathrm{e}^{-V_{\min} t}$ and behave, as a function of N, similarly to in the non-interacting case. The conditional expectations (20), which now reduce to residual canonical averages over both the variables N_T and N_V, can be evaluated analogously with equation (21). The result again implies that the saddle point integrations we perform to evaluate (i) the weights, (ii) the residual canonical averages and (iii) the sum of the series $\sum_{N=0}^{\infty} \mathsf{E}(\mathcal{M}_{\boldsymbol{n}_0}^t | N_t = N)$ all become exact in the limit $t \to \infty$. The conclusion is that for hard-core boson systems in the absence of magnetic fields, i.e. $\mathscr{L} = \{1\}$, the ground-state energy $E_{0\mathrm{B}}$ is determined by the following scalar equation involving all the cumulants of the Markov dynamics:

$$\sum_{k=1}^{\infty} \frac{1}{k!} \sum_{\alpha_1 \in \mathscr{H}} \cdots \sum_{\alpha_k \in \mathscr{H}} \Sigma_{\alpha_1,\ldots,\alpha_k}^{(k)} u_{\alpha_1}(E_{0\mathrm{B}}) \cdots u_{\alpha_k}(E_{0\mathrm{B}}) = 0 \qquad E_{0\mathrm{B}} \leq V_{\min}, \tag{24}$$

where $\mathscr{H} = \mathscr{V} \cup \mathscr{T}$, and the vector $\boldsymbol{u}^{\mathrm{T}} = (\cdots u_V \cdots ; \cdots u_T \cdots)$ with $V \in \mathscr{V}$ and $T \in \mathscr{T}$ is defined as

$$\boldsymbol{u}^{\mathrm{T}}(E_{0\mathrm{B}}) = (\cdots - \log[(-E_{0\mathrm{B}} + V)/\epsilon] \cdots ; \cdots \log T \cdots). \tag{25}$$

The existence of a unique solution of equation (24) is ensured by the condition $E_{0B} \le V_{min}$. The asymptotic rescaled cumulants $\Sigma_{\alpha_1,\dots,\alpha_k}^{(k)}$ are defined as

$$\Sigma_{\alpha_1,\dots,\alpha_k}^{(k)} = \lim_{N\to\infty} \frac{\langle N_{\alpha_1} \cdots N_{\alpha_k} \rangle_N^{(c)}}{N}, \tag{26}$$

where by $\langle \cdot \rangle_N^{(c)}$ we mean the cumulants, or connected correlation functions, of the multiplicities N_α, $\alpha \in \mathscr{H}$, sampled with respect to the measure induced at N jumps by the Markov chain with the transition matrix (16).

For $\hat{V} \equiv 0$, equation (24) can be solved explicitly and we get the following exact expression for the ground-state energy $E_{0B}^{(0)}$ of a non-interacting hard-core boson system:

$$E_{0B}^{(0)} = -\epsilon \exp\left[\sum_{k=1}^{\infty} \frac{1}{k!} \sum_{T_1 \in \mathscr{T}} \cdots \sum_{T_k \in \mathscr{T}} \Sigma_{T_1,\dots,T_k}^{(k)} \log T_1 \cdots \log T_k \right]. \tag{27}$$

For a generic $\hat{V}$, equation (24), with the series truncated at an arbitrary finite order k_{max}, can be solved numerically in a straightforward way by using the bounds $E_{0B}^{(0)} + V_{min} \le E_{0B} \le V_{min}$.

Equation (24) allows us, via the Hellmann–Feynman theorem (5), to also evaluate the expectation of any other operator in the ground state of the chosen Hamiltonian (see [5] for more details). Moreover, it is clear that the cumulants $\mathbf{\Sigma}^{(k)}$ depend only on the structure of the Hamiltonian operator, not on the values of the Hamiltonian parameters. Therefore, once the $\mathbf{\Sigma}^{(k)}$ are known, all the evaluated ground-state expectations are given analytically in terms of the Hamiltonian parameters.

Our analytical formula for the ground-state energy (24) rests on the knowledge of the asymptotic rescaled cumulants. In some special cases, it could be possible to also evaluate, at least approximatively, these cumulants analytically. We refer the reader to section 5 for a detailed discussion on determining the cumulants in a numerical way. In that section, some example cases are worked out explicitly. Finally, we refer the reader to section 6 for a scenario of possible applications that exploit the analytic character of our approach.

4. Probabilistic expectation in the long-time limit: proof of equations (24)–(27)

4.1. Canonical decomposition of the expectation

To evaluate the expectation $\mathsf{E}(\mathcal{M}_{\boldsymbol{n}_0}^t)$, we decompose it as a series of conditional expectations with a fixed number of jumps (canonical averages):

$$\mathsf{E}(\mathcal{M}_{\boldsymbol{n}_0}^t) = \sum_{N=0}^{\infty} \mathsf{E}(\mathcal{M}_{\boldsymbol{n}_0}^t | N_t = N). \tag{28}$$

In the canonical averages the stochastic jump times are easily integrated out. In fact, multiplying the stochastic functional (13) with the condition $N_t = N$ by the infinitesimal probability,

$$\mathrm{d}P_N = \mathrm{e}^{-|\Gamma|s_1} \rho \, \mathrm{d}s_1 \mathrm{e}^{-|\Gamma|(s_2 - s_1)} \rho \, \mathrm{d}s_2 \cdots \mathrm{e}^{-|\Gamma|(s_N - s_{N-1})} \rho \, \mathrm{d}s_N \, \mathrm{e}^{-|\Gamma|(t - s_N)},$$

to obtain the jumps $1, 2, \dots, N$ of the independent Poisson processes in the intervals $[s_1, s_1 + \mathrm{d}s_1), [s_2, s_2 + \mathrm{d}s_2), \dots, [s_N, s_N + \mathrm{d}s_N)$, respectively, and integrating over the times

$s_1, s_2, \ldots, s_N$, we get

$$\mathsf{E}(\mathcal{M}_{\boldsymbol{n}_0}^t | N_t = N) = \sum_{r \in \Omega_N} \mathcal{S}_N^{(r)} \mathcal{K}_N^{(r)} \mathcal{W}_N^{(r)}(t), \tag{29}$$

where $\Omega_N = \Omega_N(\boldsymbol{n}_0)$ is the set of all possible trajectories with N jumps branching from the initial configuration $\boldsymbol{n}_0$ and

$$\mathcal{S}_N^{(r)} = \lambda_1^{(r)} \lambda_2^{(r)} \cdots \lambda_N^{(r)}, \tag{30}$$

$$\mathcal{K}_N^{(r)} = \epsilon^{-N} \eta_1^{(r)} \eta_2^{(r)} \cdots \eta_N^{(r)}, \tag{31}$$

$$\mathcal{W}_N^{(r)}(t) = \epsilon^N \int_0^t \mathrm{d}s_1 \int_{s_1}^t \mathrm{d}s_2 \cdots \int_{s_{N-1}}^t \mathrm{d}s_N \, \mathrm{e}^{-V_0 s_1 - V_1^{(r)}(s_2 - s_1) \cdots - V_N^{(r)}(t - s_N)}. \tag{32}$$

Equations (30), (31) and (32) define three dimensionless quantities related, respectively, to the sequences of the signs (more generally, of the phases) of the hopping parameters and of the potential values associated with the rth trajectory with $N > 0$ jumps. We have $\mathcal{S}_0^{(r)} = \mathcal{K}_0^{(r)} = 1$ and $\mathcal{W}_0^{(r)}(t) = \mathrm{e}^{-V_0 t}$ in the case $N = 0$. The quantities $\mathcal{W}_N^{(r)}(t)$ are positive definite and will be called weights in the following.

From equation (30), it is clear that only the trajectories formed by a sequence of active links contribute to the sum in equation (29). Hereafter, therefore, we restrict Ω_N to being the set of these effective trajectories with N jumps branching from $\boldsymbol{n}_0$ and we exclude the value $\lambda = 0$ from the set $\mathscr{L}$.

The sum over the set Ω_N can be expressed as an average, $\langle \cdot \rangle_N$, over the trajectories with N jumps generated by extracting with uniform probability one of the active links available at the configurations $\boldsymbol{n}_0, \boldsymbol{n}_1, \ldots, \boldsymbol{n}_{N-1}$. The probability associated with the rth trajectory generated in this way is $p_N^{(r)} = \prod_{k=0}^{N-1} 1/A_k^{(r)}$ and we have

$$\sum_{r \in \Omega_N} \mathcal{S}_N^{(r)} \mathcal{K}_N^{(r)} \mathcal{W}_N^{(r)}(t) = \sum_{r \in \Omega_N} p_N^{(r)} \mathcal{S}_N^{(r)} \mathcal{K}_N^{(r)} \mathcal{W}_N^{(r)}(t) \prod_{k=0}^{N-1} A_k^{(r)} = \left\langle \mathcal{S}_N \mathcal{W}_N(t) \prod_{k=0}^{N-1} T_k \right\rangle_N, \tag{33}$$

where $\langle \cdot \rangle_N = \sum_{r \in \Omega_N} \cdot \, p_N^{(r)}$. Note that $\sum_{r \in \Omega_N} p_N^{(r)} = 1$. By using the definitions (18a) and (18c), we rewrite the canonical averages as

$$\mathsf{E}(\mathcal{M}_{\boldsymbol{n}_0}^t | N_t = N) = \left\langle \mathcal{W}_N(t) \prod_{\lambda \in \mathscr{L}} \lambda^{N_\lambda} \prod_{T \in \mathscr{T}} T^{N_T} \right\rangle_N. \tag{34}$$

In the following, we will consider only hard-core bosons in the absence of magnetic fields. In this case, $\mathscr{L} = \{1\}$ and we are left with averages of positive definite quantities:

$$\mathsf{E}(\mathcal{M}_{\boldsymbol{n}_0}^t | N_t = N) = \left\langle \mathcal{W}_N(t) \prod_{T \in \mathscr{T}} T^{N_T} \right\rangle_N. \tag{35}$$

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4.2. Evaluation of the weights

In this section, first we find a recursive differential equation for the weights $\mathcal{W}_N(t)$. Then, taking the Laplace transform of this equation, we realize that the weights depend only on the multiplicities N_V of the potential, not on the detailed sequence $V_0, V_1, \ldots, V_N$. Finally, we use a saddle point technique on the complex plane to obtain an explicit expression for the weights, which becomes exact in the limit $N \to \infty$.

Equation (32), which defines the weights $\mathcal{W}_N(t)$ for $N \geq 1$, can be rewritten as (for simplicity, we omit the trajectory index (r) but we stress the dependence on the sequence of the potential values)

$$\mathcal{W}_N(t; V_0, V_1, \ldots, V_N) = G_N(t; V_0, V_1, \ldots, V_N)\mathrm{e}^{-V_N t},$$

where

$$G_N(t; V_0, V_1, \ldots, V_N) = \epsilon^N \int_0^t \mathrm{d}s_1 \int_0^t \mathrm{d}s_2 \cdots \int_0^t \mathrm{d}s_N\, \theta(s_2 - s_1)\theta(s_3 - s_2) \cdots$$
$$\times\, \theta(s_N - s_{N-1}) \exp(\Delta_1 s_1 + \Delta_2 s_2 + \cdots + \Delta_N s_N),$$

with $\Delta_k = V_k - V_{k-1}$, $k = 1, 2, \ldots, N$. By evaluating the derivative of $G_N(t)$, for $N > 0$, with respect to t,

$$\partial_t G_N(t; V_0, V_1, \ldots, V_N) = \epsilon G_{N-1}(t; V_0, V_1, \ldots, V_{N-1}) \exp(\Delta_N t),$$

where $G_0(t; V_0) = 1$, we find the following recursive ordinary differential equation for $\mathcal{W}_N(t)$:

$$\partial_t \mathcal{W}_N(t; V_0, V_1, \ldots, V_N) = \epsilon \mathcal{W}_{N-1}(t; V_0, V_1, \ldots, V_{N-1}) - V_N \mathcal{W}_N(t; V_0, V_1, \ldots, V_N). \tag{36}$$

Since equation (36) is linear in $\mathcal{W}_N(t)$ and $\mathcal{W}_{N-1}(t)$, it is convenient to introduce the Laplace transform

$$\tilde{\mathcal{W}}_N(z) = \int_0^\infty \mathrm{d}t\, \mathrm{e}^{-zt} \mathcal{W}_N(t), \qquad z \in \mathbb{C}.$$

On observing that $\mathcal{W}_N(0) = 0$ for $N > 0$, equation (36) reduces to the following recursive algebraic equation for $\tilde{\mathcal{W}}_N(z)$:

$$z\tilde{\mathcal{W}}_N(z) = \epsilon \tilde{\mathcal{W}}_{N-1}(z) - V_N \tilde{\mathcal{W}}_N(z), \tag{37}$$

from which we get

$$\tilde{\mathcal{W}}_N(z) = \epsilon(z + V_N)^{-1} \tilde{\mathcal{W}}_{N-1}(z). \tag{38}$$

We recall that for $N = 0$ we have $\mathcal{W}_0(t; V_0) = \mathrm{e}^{-V_0 t}$ and, therefore, $\tilde{\mathcal{W}}_0(z) = (z + V_0)^{-1}$. By iterating equation (38), we arrive at the solution

$$\tilde{\mathcal{W}}_N(z) = \epsilon^N \prod_{k=0}^N \frac{1}{z + V_k},$$

which, in terms of the multiplicities (18b), takes the form

$$\tilde{\mathcal{W}}_N(z) = \epsilon^N \prod_{V \in \mathscr{V}} (z + V)^{-N_V}. \tag{39}$$

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This expression shows that, for any value of N, the weights depend only on the multiplicities N_V, i.e. $\mathcal{W}_N(t; V_0, V_1, \ldots, V_N) = \mathcal{W}_N(t; \{N_V\})$.

The explicit inversion of the Laplace transform (39) can be done analytically only for N large. However, as we will immediately prove, this is the limit we are interested in. In fact, in the case $\hat{V} \equiv 0$, we have $\mathcal{W}_N(t) = \mathcal{W}_N^{(0)}(t) = \epsilon^N t^N / N!$, which is easily obtained by direct integration of equation (32). For t large $\mathcal{W}_N^{(0)}(t)$ has, as a function of N, a maximum at $N(t) = \epsilon t$ and, around this maximum, is well approximated by a Gaussian of width $\sqrt{N(t)}$. For $\hat{V}$ generic, let us indicate by $V_{\min}$ and $V_{\max}$ the minimum and maximum elements of $\mathscr{V}$ such that $N_V \neq 0$ for the trajectory we are considering. In equation (32) we thus have $V_{\min} \leq V_k \leq V_{\max}$, $k = 0, 1, \ldots, N$, and

$$\mathrm{e}^{-V_{\max}t} \leq \mathrm{e}^{-V_0 s_1 - V_1(s_2 - s_1)\cdots - V_N(t - s_N)} \leq \mathrm{e}^{-V_{\min}t}. \tag{40}$$

We conclude that the weights are bounded by

$$\mathcal{W}_N^{(0)}(t)\mathrm{e}^{-V_{\max}t} \leq \mathcal{W}_N(t) \leq \mathcal{W}_N^{(0)}(t)\mathrm{e}^{-V_{\min}t}, \tag{41}$$

so that, for $t \to \infty$, exponentially leading contributions are obtained from values of N in the range $[\epsilon t - \sqrt{\epsilon t}, \epsilon t + \sqrt{\epsilon t}]$.

According to equation (39), $\tilde{\mathcal{W}}_N(z)$ has $m_N \leq m_{\mathscr{V}}$ poles at the points $z_V = -V$ such that $V \in \mathscr{V}$ and $N_V \neq 0$. For N sufficiently large, the number m_N of these poles approaches $m_{\mathscr{V}}$. For any finite value of N, the poles of $\tilde{\mathcal{W}}_N(z)$ are confined in the real segment $[-V_{\max}, -V_{\min}]$. Recalling the rule for the Laplace inverse transformation, we have

$$\mathcal{W}_N(t) = \frac{1}{2\pi\mathrm{i}} \int_{\Gamma} \mathrm{d}z\, \mathrm{e}^{zt} \tilde{\mathcal{W}}_N(z),$$

where the integration contour Γ can be any line parallel to the imaginary axis and contained in the analyticity domain of the Laplace transform. In our case, Γ must be in the domain $\mathrm{Re}\, z > -V_{\min}$. By Jordan's lemma, the contour can be closed to infinity in the left half-plane $\mathrm{Re}\, z < -V_{\min}$ without changing the integration result. Finally, by Cauchy's theorem, Γ can be deformed into any other anticlockwise closed contour Γ' still containing all the poles z_V.

Using the expression (39) for $\tilde{\mathcal{W}}_N(z)$, we write its anti-transform as

$$\mathcal{W}_N(t) = \frac{1}{2\pi\mathrm{i}\epsilon} \int_{\Gamma} \mathrm{d}z\, \exp[N\varphi(z)], \tag{42}$$

where

$$\varphi(z) = \frac{zt}{N} - \sum_{V \in \mathscr{V}} \frac{N_V}{N} \log \frac{z + V}{\epsilon}. \tag{43}$$

For t large and $N \sim t$, since also $N_V \sim N$ due to the ergodicity of the trajectories, we can evaluate the complex integral (42) by a saddle point technique. Let us call the point of the complex plane where $\varphi(z)$ is stationary z_0, i.e. $\partial_z \varphi(z_0) = 0$. We deform the contour Γ into a new one, Γ' (steepest descent), such that, for $z \in \Gamma'$, $\mathrm{Re}\, \varphi(z)$ has a maximum at z_0, whereas $\mathrm{Im}\, \varphi(z)$ is constant, at least at the first order in its Taylor expansion around z_0. Provided that the contour Γ' remains in the analyticity domain of $\varphi(z)$, the following

standard result applies [10]:

$$\mathcal{W}_N(t) = \frac{1}{2\pi i \epsilon} \sqrt{\frac{2\pi}{N|\partial_z^2 \varphi(z_0)|}} \exp[i\alpha + N\varphi(z_0)], \tag{44}$$

where α is defined as

$$\alpha = \frac{\pi}{2} - \frac{1}{2} \arg \partial_z^2 \varphi(z_0) \tag{45}$$

and represents the angle formed, at the saddle point z_0, by the new contour Γ' with respect to the original one Γ.

Now we calculate the first and second derivatives of $\varphi(z)$ and the saddle point z_0. From equation (43) we have

$$\partial_z \varphi(z) = \frac{t}{N} - \sum_{V \in \mathscr{V}} \frac{N_V}{N} \frac{1}{z+V}, \tag{46}$$

$$\partial_z^2 \varphi(z) = \sum_{V \in \mathscr{V}} \frac{N_V}{N} \frac{1}{(z+V)^2}. \tag{47}$$

In terms of $x_0 = \operatorname{Re} z_0$ and $y_0 = \operatorname{Im} z_0$, the saddle point equation, $\partial_z \varphi(z_0) = 0$, reads

$$\frac{t}{N} - \sum_{V \in \mathscr{V}} \frac{N_V}{N} \frac{x_0}{(x_0+V)^2 + y_0^2} = 0, \tag{48a}$$

$$\sum_{V \in \mathscr{V}} \frac{N_V}{N} \frac{y_0}{(x_0+V)^2 + y_0^2} = 0. \tag{48b}$$

As $N_V \geq 0$, equation (48b) is satisfied only by $y_0 = 0$. Hence, we are left with the following equation for x_0:

$$\sum_{V \in \mathscr{V}} \frac{N_V}{x_0 + V} = t. \tag{49}$$

For any $t > 0$, equation (49) has m_N solutions. The first $m_N - 1$ solutions, ordered according to increasing value, are in the range $-V_{\max} < x_0 < -V_{\min}$, whereas the last one is such that $x_0 > -V_{\min}$. This is the only solution compatible with the condition that the integration contour Γ, passing through $z_0 = x_0 + iy_0$, is contained in the analyticity domain of $\varphi(z)$. Therefore, for any $t > 0$, we have one and only one saddle point determined by equation (49) with the constraint $x_0 > -V_{\min}$.

The fact that $y_0 = 0$ also implies

$$\partial_z^2 \varphi(z_0) = \sum_{V \in \mathscr{V}} \frac{N_V}{N} \frac{1}{(x_0 + V)^2}, \tag{50}$$

so that we have

$$\arg \partial_z^2 \varphi(z_0) = 0, \tag{51}$$

i.e. $\alpha = \pi/2$. The integration contour Γ, therefore, has to be deformed into a new one Γ' parallel to the real axis. At a first sight, this kind of deformation is incompatible with the condition that Γ' strictly contains all the poles z_V located on the real axis. However,
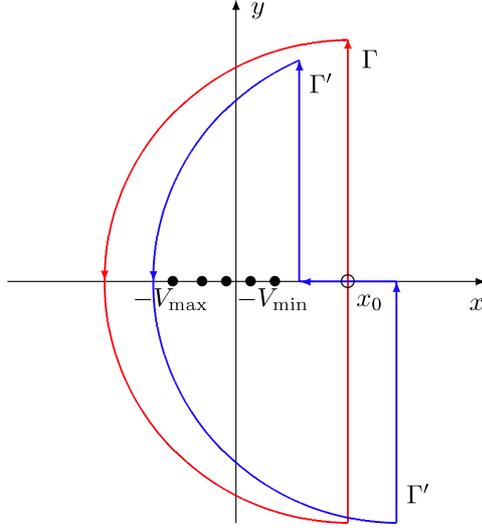
Figure 1. Integration contours Γ and Γ' in the complex plane $z = x + \mathrm{i}y$, which are used to evaluate the Laplace anti-transform of $\tilde{\mathcal{W}}_N(z)$. The saddle point x_0 and the poles of $\tilde{\mathcal{W}}_N(z)$ are indicated by open and filled circles, respectively.

the largest solution of equation (49) is bounded from below by $x_0 > -V_{\min} + N_{V_{\min}}/t$. This means that for $t \to \infty$ with $N_{V_{\min}} \sim N \sim t$, the distance between the saddle point and the closest pole at $z = -V_{\min}$ is finite. Therefore, we can take Γ' parallel to the real axis only in a finite neighbourhood of the saddle point as shown in figure 1. In fact, the contribution to the integral due to this neighbourhood of z_0 is exponentially leading in N with respect to the rest of the contour.

In conclusion, for $t \to \infty$ with $N \sim t$, the integration on the contour Γ' chosen as described above becomes asymptotically exact and, in this limit, we have the following exact expression for the weights:

$$\mathcal{W}_N(t) = \frac{\mathrm{e}^{x_0 t - \sum_{V \in \mathscr{V}} N_V \log[(x_0 + V)/\epsilon]}}{\sqrt{2\pi \sum_{V \in \mathscr{V}} (\epsilon^2 N_V/(x_0 + V)^2)}}, \tag{52a}$$

$$\sum_{V \in \mathscr{V}} \frac{N_V}{x_0 + V} = t, \qquad x_0 > -V_{\min}. \tag{52b}$$

This expression is semi-analytic in the sense that the simple equation (52b), which provides x_0 to be inserted into equation (52a), must be solved, in general, numerically or recursively.

For $\check{V} \equiv 0$, we can verify that the above expression for the weights reproduces the exact result $\mathcal{W}_N^{(0)}(t) = \epsilon^N t^N/N!$. In this case $\mathscr{V} = \{0\}$ and the solution of equation (52b) is

$$x_0 = \frac{N+1}{t}. \tag{53}$$

Inserting this value into equation (52a), we have

$$\mathcal{W}_N^{(0)}(t) = \frac{\exp[N + 1 - (N+1)\log[(N+1)/\epsilon t]]}{\sqrt{2\pi\epsilon^2 t^2/(N+1)}}$$

$$= \frac{1}{\sqrt{2\pi}} \frac{\exp(N+1)}{(N+1)^{N+1/2}} \epsilon^N t^N. \tag{54}$$

On recalling Stirling's formula

$$N! \simeq \sqrt{2\pi} N^{N+1/2} \mathrm{e}^{-N}, \tag{55}$$

which derives from a saddle point evaluation of the Gamma function as well, we see that equation (54) is just the Stirling approximation to $\epsilon^N t^N / N!$.

4.3. Canonical averages via large deviation analysis

To evaluate the canonical averages it is useful to introduce the frequencies, $\nu_V = N_V/N$, $V \in \mathscr{V}$ and $\nu_T = N_T/N$, $T \in \mathscr{T}$, which for N large become continuously distributed in the range $[0,1]$ with the constraints

$$\sum_{V \in \mathscr{V}} \nu_V = \sum_{T \in \mathscr{T}} \nu_T = 1. \tag{56}$$

Note that, for N large, we do not distinguish the different normalizations, $N+1$ and N, of N_V and N_T, respectively. When possible, we will use a compact notation in terms of the vectors $\boldsymbol{\mu}$ and $\boldsymbol{\nu}$, which have $m = m_{\mathscr{V}} + m_{\mathscr{T}}$ components indicated by a Greek index $\alpha \in \mathscr{H} = \mathscr{V} \cup \mathscr{T}$ and are defined as $\boldsymbol{\mu}^{\mathrm{T}} = (\cdots N_V \cdots; \cdots N_T \cdots)$ and $\boldsymbol{\nu}^{\mathrm{T}} = (\cdots \nu_V \cdots; \cdots \nu_T \cdots)$. We have

$$\boldsymbol{\mu} = N\boldsymbol{\nu}. \tag{57}$$

For later use, we also define $\boldsymbol{u}^{\mathrm{T}} = (\cdots - \log[(x_0 + V)/\epsilon] \cdots; \cdots \log T \cdots)$, $\boldsymbol{v}^{\mathrm{T}} = (\cdots (x_0 + V)^{-1} \cdots; \cdots 0 \cdots)$ and $\boldsymbol{w}^{\mathrm{T}} = (\cdots (x_0 + V)^{-2} \cdots; \cdots 0 \cdots)$. Note that the vectors $\boldsymbol{u}$, $\boldsymbol{v}$ and $\boldsymbol{w}$ depend on $\boldsymbol{\nu}$ through $x_0 = x_0(\boldsymbol{\nu})$ and $\boldsymbol{v} = -\partial_{x_0} \boldsymbol{u}$, $\boldsymbol{w} = -\partial_{x_0} \boldsymbol{v}$. Finally, we will take advantage of a scalar product notation. For instance, we rewrite the saddle point equation (52b) as $(\boldsymbol{\nu}, \boldsymbol{v}) = t/N$.

Using the result given by equations (52a) and (52b), we express the rhs of equation (35) in the following explicit form:

$$\left\langle \mathcal{W}_N(t) \prod_{T \in \mathscr{T}} T^{N_T} \right\rangle_N = \sum_{\boldsymbol{\mu}} \mathcal{P}_N(\boldsymbol{\mu}) \frac{\mathrm{e}^{x_0 t + (\boldsymbol{\mu}, \boldsymbol{u})}}{\sqrt{2\pi \epsilon^2 (\boldsymbol{\mu}, \boldsymbol{w})}}. \tag{58}$$

The probability $\mathcal{P}_N(\boldsymbol{\mu})$ is given by the fraction of trajectories branching from the initial configuration $\boldsymbol{n}_0$ and having after N jumps multiplicities $\boldsymbol{\mu}$. According to Poisson's summation formula

$$\sum_{\boldsymbol{\mu}} f(\boldsymbol{\mu}) = \sum_{\boldsymbol{k} \in \mathbb{Z}^m} \int \mathrm{d}\boldsymbol{\mu} \, \mathrm{e}^{\mathrm{i}(\boldsymbol{k}, \boldsymbol{\mu})} f(\boldsymbol{\mu}), \tag{59}$$

the sum over $\boldsymbol{\mu}$ in equation (58) can be transformed into a series for $\boldsymbol{k} \in \mathbb{Z}^m$ of integrals over the same variable in the presence of the oscillating factors $\exp[\mathrm{i}(\boldsymbol{k}, \boldsymbol{\mu})]$. As we will check at the end of the calculation, in the limit of t large all the terms $\boldsymbol{k} \neq \boldsymbol{0}$ of this series are exponentially damped with respect to the term $\boldsymbol{k} = \boldsymbol{0}$. In this limit, therefore, we will not distinguish the sum over $\boldsymbol{\mu}$ in equation (58) from the corresponding integral.

In [5] we have evaluated equation (58) for t large by using a central limit theorem for Markov chains. Although this theorem applies rigorously to each rescaled sum $N_\alpha/\sqrt{N} = \nu_\alpha \sqrt{N}$, $\alpha \in \mathscr{H}$, it provides an approximation when, as in equation (58), variables like $\nu_\alpha N$ are involved. As anticipated in [5], the integrand in equation (58) is

sensitive to the large deviations of $\mathcal{P}_N(\boldsymbol{\mu})$ from the central limit behaviour and to obtain more accurate estimates we need to consider a development in terms of the associated cumulants (connected correlation functions) [8].

Before proceeding with this analysis, we observe that the constraints (56) give important summation rules for the cumulants. Let us indicate by $\langle \nu_{\alpha_1} \cdots \nu_{\alpha_k} \rangle_N^{(c)}$, $\alpha_1, \ldots, \alpha_k \in \mathscr{H}$, a cumulant of order k. In appendix A, we demonstrate that

$$\sum_{\alpha \in \mathscr{V}} \langle \nu_\alpha \rangle_N^{(c)} = \sum_{\alpha \in \mathscr{T}} \langle \nu_\alpha \rangle_N^{(c)} = 1, \tag{60}$$

for $k = 1$, whereas for $k > 1$

$$\sum_{\alpha_k \in \mathscr{V}} \langle \nu_{\alpha_1} \cdots \nu_{\alpha_k} \rangle_N^{(c)} = \sum_{\alpha_k \in \mathscr{T}} \langle \nu_{\alpha_1} \cdots \nu_{\alpha_k} \rangle_N^{(c)} = 0. \tag{61}$$

These rules provide a basic test for the statistical measurement of the cumulants themselves. A sampling that aims at measuring the cumulants with a given accuracy will have to satisfy equations (60) and (61) with the same accuracy.

As is customary in the framework of a large deviation analysis, we are interested in getting information about the density $\mathcal{P}_N(N\boldsymbol{\nu})$ in the limit of N large and $\boldsymbol{\nu}$ finite. On introducing the Fourier anti-transformation

$$\mathcal{P}_N(\boldsymbol{\mu}) = \frac{1}{(2\pi)^m} \int \mathrm{d}\boldsymbol{q}\, \mathrm{e}^{\log[\tilde{\mathcal{P}}_N(\boldsymbol{q})] - \mathrm{i}(\boldsymbol{q}, \boldsymbol{\mu})}, \tag{62}$$

$\tilde{\mathcal{P}}_N(\boldsymbol{q})$ being the Fourier transform of $\mathcal{P}_N(\boldsymbol{\mu})$, equation (58) becomes

$$\left\langle \mathcal{W}_N(t) \prod_{T \in \mathscr{T}} T^{N_T} \right\rangle_N = \left(\frac{N}{2\pi} \right)^m \int \mathrm{d}\boldsymbol{\nu} \int \mathrm{d}\boldsymbol{q}\, \mathrm{e}^{N\phi(\boldsymbol{\nu}, \boldsymbol{q})} R(\boldsymbol{\nu}), \tag{63}$$

where $\phi(\boldsymbol{\nu}, \boldsymbol{q})$ takes into account the exponential behaviour of the integrand, whereas $R(\boldsymbol{\nu})$ is a smooth function. For brevity, we omit the parametric dependence of ϕ and R on t and N. Explicitly, we have

$$\phi(\boldsymbol{\nu}, \boldsymbol{q}) = x_0 \frac{t}{N} + (\boldsymbol{\nu}, \boldsymbol{u}) - \mathrm{i}(\boldsymbol{\nu}, \boldsymbol{q}) + \frac{\log \tilde{\mathcal{P}}_N(\boldsymbol{q})}{N} \tag{64}$$

$$R(\boldsymbol{\nu}) = \frac{1}{\sqrt{2\pi N \epsilon^2(\boldsymbol{\nu}, \boldsymbol{w})}}. \tag{65}$$

As is well known, the cumulants are related to $\log \tilde{\mathcal{P}}_N(\boldsymbol{q})$ through the relation

$$\begin{aligned}
\log \tilde{\mathcal{P}}_N(\boldsymbol{q}) &= \log \langle \mathrm{e}^{\mathrm{i}(\boldsymbol{\mu}, \boldsymbol{q})} \rangle_N, \\
&= \sum_{k=1}^{\infty} \frac{1}{k!} \langle (\boldsymbol{\mu}, \mathrm{i}\boldsymbol{q})^k \rangle_N^{(c)}, \\
&= \sum_{k=1}^{\infty} \frac{N^k}{k!} \langle (\boldsymbol{\nu}, \mathrm{i}\boldsymbol{q})^k \rangle_N^{(c)}.
\end{aligned} \tag{66}$$

Note that for any given N, due to the inequalities $\langle \mu_{\alpha_1} \cdots \mu_{\alpha_k} \rangle_N \leq N^k$, valid for any k, and due to the asymmetry $\mathcal{P}_N(\boldsymbol{\mu}) \neq \mathcal{P}_N(-\boldsymbol{\mu})$, the series in equation (66) converge for every $\boldsymbol{q} \in \mathbb{C}^m$ (see, for example, [8]).

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We evaluate the integrals in equation (63) by a saddle point calculation (actually Laplace's method) with respect to the variable $(\boldsymbol{\nu}, \boldsymbol{q}) \in \mathbb{R}^m \times \mathbb{R}^m$. The derivatives of $\phi(\boldsymbol{\nu}, \boldsymbol{q})$ with respect to q_α and ν_α, $\alpha \in \mathscr{H}$, are

$$\partial_{q_\alpha}\phi(\boldsymbol{\nu}, \boldsymbol{q}) = \mathrm{i}\sum_{k=1}^{\infty} \frac{N^{k-1}}{(k-1)!}\langle(\boldsymbol{\nu}, \mathrm{i}\boldsymbol{q})^{k-1}\nu_\alpha\rangle_N^{(c)} - \mathrm{i}\nu_\alpha$$

$$\partial_{\nu_\alpha}\phi(\boldsymbol{\nu}, \boldsymbol{q}) = -\mathrm{i}q_\alpha + u_\alpha,$$

where we have used $(\boldsymbol{\nu}, \boldsymbol{v}) = t/N$. Therefore, the stationarity condition for $\phi(\boldsymbol{\nu}, \boldsymbol{q})$ implies

$$\nu_\alpha = \sum_{k=1}^{\infty} \frac{N^{k-1}}{(k-1)!}\langle(\boldsymbol{\nu}, \mathrm{i}\boldsymbol{q})^{k-1}\nu_\alpha\rangle_N^{(c)}$$

$$\mathrm{i}q_\alpha = u_\alpha,$$

which, in turn, reduces to the following equation for the saddle point frequencies $\boldsymbol{\nu}^{\mathrm{sp}}$:

$$\nu_\alpha^{\mathrm{sp}} = \sum_{k=1}^{\infty} \frac{N^{k-1}}{(k-1)!}\langle(\boldsymbol{\nu}, \boldsymbol{u}(x_0(\boldsymbol{\nu}^{\mathrm{sp}})))^{k-1}\nu_\alpha\rangle_N^{(c)}. \tag{67}$$

Hereafter, we will add the superscript $^{\mathrm{sp}}$ to a function of $\boldsymbol{\nu}$ to indicate the value of this function for $\boldsymbol{\nu} = \boldsymbol{\nu}^{\mathrm{sp}}$. On approximating the function $\phi(\boldsymbol{\nu}, \boldsymbol{q})$ with its second-order Taylor expansion around the saddle point $(\boldsymbol{\nu}^{\mathrm{sp}}, \boldsymbol{q}^{\mathrm{sp}})$ and performing the resulting Gaussian integral with respect to the variable $(\boldsymbol{\nu} - \boldsymbol{\nu}^{\mathrm{sp}}, \boldsymbol{q} - \boldsymbol{q}^{\mathrm{sp}})$, equation (63) becomes

$$\left\langle \mathcal{W}_N(t) \prod_{T \in \mathscr{T}} T^{N_T} \right\rangle_N = C_N \exp\left[\psi(N)\right], \tag{68}$$

where

$$\psi(N) = N\phi(\boldsymbol{\nu}^{\mathrm{sp}}, \boldsymbol{q}^{\mathrm{sp}})$$

$$= x_0^{\mathrm{sp}}t + N\sum_{k=1}^{\infty} \frac{N^{k-1}}{k!}\langle(\boldsymbol{\nu}, \boldsymbol{u}^{\mathrm{sp}})^k\rangle_N^{(c)} \tag{69}$$

$$C_N = \frac{R(\boldsymbol{\nu}^{\mathrm{sp}})}{\sqrt{|\det \nabla^2\phi(\boldsymbol{\nu}^{\mathrm{sp}}, \boldsymbol{q}^{\mathrm{sp}})|}}, \tag{70}$$

$\nabla^2\phi(\boldsymbol{\nu}, \boldsymbol{q})$ being the Jacobian of ϕ with elements

$$\partial_{q_\alpha}\partial_{q_\beta}\phi(\boldsymbol{\nu}, \boldsymbol{q}) = -\sum_{k=2}^{\infty} \frac{N^{k-1}}{(k-2)!}\langle(\boldsymbol{\nu}, \mathrm{i}\boldsymbol{q})^{k-2}\nu_\alpha\nu_\beta\rangle_N^{(c)}$$

$$\partial_{\nu_\alpha}\partial_{\nu_\beta}\phi(\boldsymbol{\nu}, \boldsymbol{q}) = -\frac{v_\alpha v_\beta}{(\boldsymbol{\nu}, \boldsymbol{w})}$$

$$\partial_{q_\alpha}\partial_{\nu_\beta}\phi(\boldsymbol{\nu}, \boldsymbol{q}) = \partial_{\nu_\alpha}\partial_{q_\beta}\phi(\boldsymbol{\nu}, \boldsymbol{q}) = -\mathrm{i}\delta_{\alpha,\beta},$$

for $\alpha, \beta \in \mathscr{H}$. It is convenient to introduce two $m \times m$ matrices $\boldsymbol{\Sigma}$ and $\boldsymbol{A}$ with elements

$$\Sigma_{\alpha,\beta} = -\partial_{q_\alpha}\partial_{q_\beta}\phi(\boldsymbol{\nu}^{\mathrm{sp}}, \boldsymbol{q}^{\mathrm{sp}}) \tag{71}$$

$$A_{\alpha,\beta} = -\partial_{\nu_\alpha}\partial_{\nu_\beta}\phi(\boldsymbol{\nu}^{\mathrm{sp}}, \boldsymbol{q}^{\mathrm{sp}}). \tag{72}$$

In terms of these matrices equation (70) becomes

$$C_N = \frac{1}{\sqrt{|\det(\mathbf{1} + \mathbf{\Sigma A})|}} \frac{1}{\sqrt{2\pi N \epsilon^2 (\boldsymbol{\nu}^{\mathrm{sp}}, \boldsymbol{w}^{\mathrm{sp}})}}. \tag{73}$$

Note that, in the case $\hat{V} \equiv 0$, the matrix $\boldsymbol{A}$ is uniform and, due to the summation rules (60) and (61), $\mathbf{\Sigma A} = \mathbf{0}$. In general, the same summation rules imply $\det(\mathbf{\Sigma A}) = 0$, so that $\det(\mathbf{1} + \mathbf{\Sigma A}) \simeq 1$ up to second-order terms in $\boldsymbol{A}$.

4.4. Resumming the canonical series

In this section, we evaluate the expectation $\mathsf{E}(\mathcal{M}_{\boldsymbol{n}_0}^t)$ by resumming the series of equation (28). We will replace the series over N by the integral

$$\mathsf{E}(\mathcal{M}_{\boldsymbol{n}_0}^t) = \int \mathrm{d}N \, C_N \exp[\psi(N)], \tag{74}$$

and we will perform the integration again with a saddle point technique. At the end, we will demonstrate the asymptotic exactness, in the limit $t \to \infty$, of the saddle point integration, as well as of the substitution of the series with the corresponding integral, by showing that in this limit equation (74) takes exponentially leading contributions from values of N in the range $[\epsilon t - \sqrt{\epsilon t}, \epsilon t + \sqrt{\epsilon t}]$.

Before evaluating the stationarity condition for $\psi(N)$, an important comment is in order. For any finite value of N, let us introduce the rescaled cumulants of order k, in a compact notation $\mathbf{\Sigma}^{(N;k)}$, which is defined as the tensor of rank k with components

$$\Sigma_{\alpha_1,\ldots,\alpha_k}^{(N;k)} = N^{k-1} \langle \nu_{\alpha_1} \cdots \nu_{\alpha_k} \rangle_N^{(c)}, \tag{75}$$

$\alpha_1, \ldots, \alpha_k \in \mathscr{H}$. Let $\mathbf{\Sigma}^{(k)}$ be the tensor of the asymptotic values of the rescaled cumulants in the limit $N \to \infty$:

$$\Sigma_{\alpha_1,\ldots,\alpha_k}^{(k)} = \lim_{N\to\infty} N^{k-1} \langle \nu_{\alpha_1} \cdots \nu_{\alpha_k} \rangle_N^{(c)} = \lim_{N\to\infty} \frac{1}{N} \langle N_{\alpha_1} \cdots N_{\alpha_k} \rangle_N^{(c)}. \tag{76}$$

These limits exist and are finite since the irreducible and finite Markov chain formed by the evolving configurations has a finite correlation length N_{c} with respect to the number of jumps (see equation (23)). Up to corrections exponentially small in N/N_{c}, for $N \gg N_{\mathrm{c}}$ we can use the effective rule

$$\partial_N \Sigma_{\alpha_1,\ldots,\alpha_k}^{(N;k)} = 0. \tag{77}$$

Using the rule (77), the derivative of $\psi(N)$ with respect to N is

$$\partial_N \psi(N) = \sum_{k=1}^{\infty} \frac{N^{k-1}}{k!} \langle (\boldsymbol{\nu}, \boldsymbol{u}^{\mathrm{sp}})^k \rangle_N^{(c)} + \partial_N x_0^{\mathrm{sp}} \left[t - N \sum_{k=1}^{\infty} \frac{N^{k-1}}{(k-1)!} \langle (\boldsymbol{\nu}, \boldsymbol{u}^{\mathrm{sp}})^{k-1} (\boldsymbol{\nu}, \boldsymbol{v}^{\mathrm{sp}}) \rangle_N^{(c)} \right].$$

On the other hand, from equation (67) we have

$$\sum_{k=1}^{\infty} \frac{N^{k-1}}{(k-1)!} \langle (\boldsymbol{\nu}, \boldsymbol{u}^{\mathrm{sp}})^{k-1} (\boldsymbol{\nu}, \boldsymbol{v}^{\mathrm{sp}}) \rangle_N^{(c)} = (\boldsymbol{\nu}^{\mathrm{sp}}, \boldsymbol{v}^{\mathrm{sp}}),$$

so that, by using $N(\boldsymbol{\nu}^{\mathrm{sp}}, \boldsymbol{v}^{\mathrm{sp}}) = t$, we find

$$\partial_N \psi(N) = \sum_{k=1}^{\infty} \frac{N^{k-1}}{k!} \langle (\boldsymbol{\nu}, \boldsymbol{u}^{\mathrm{sp}})^k \rangle_N^{(c)}. \tag{78}$$

In conclusion, the stationarity condition, $\partial_N \psi(N^{\mathrm{sp}}) = 0$, gives

$$\sum_{k=1}^{\infty} \frac{N^{k-1}}{k!} \langle (\boldsymbol{\nu}, \boldsymbol{u}^{\mathrm{sp}})^k \rangle_N^{(c)} \bigg|_{N=N^{\mathrm{sp}}} = 0, \tag{79}$$

which in terms of the rescaled cumulants (75) reads

$$\sum_{k=1}^{\infty} \frac{1}{k!} \sum_{\alpha_1 \in \mathscr{H}} \cdots \sum_{\alpha_k \in \mathscr{H}} \Sigma_{\alpha_1, \ldots, \alpha_k}^{(N;k)} u_{\alpha_1}^{\mathrm{sp}} \cdots u_{\alpha_k}^{\mathrm{sp}} \bigg|_{N=N^{\mathrm{sp}}} = 0. \tag{80}$$

Equation (80) determines the saddle point N^{sp} for the chosen value of the time t.

From equation (78) and using the rule (77), for the second derivative of $\psi(N)$ we find

$$\partial_N^2 \psi(N) = -(\boldsymbol{\nu}^{\mathrm{sp}}, \boldsymbol{v}^{\mathrm{sp}}) \partial_N x_0^{\mathrm{sp}}, \tag{81}$$

where

$$\partial_N x_0^{\mathrm{sp}} = \frac{1}{N} \frac{(\boldsymbol{\nu}^{\mathrm{sp}}, \boldsymbol{v}^{\mathrm{sp}})}{(\boldsymbol{\nu}^{\mathrm{sp}}, \boldsymbol{w}^{\mathrm{sp}}) + (\boldsymbol{\Sigma} \boldsymbol{v}^{\mathrm{sp}}, \boldsymbol{v}^{\mathrm{sp}})}. \tag{82}$$

Equation (82) has been obtained by evaluating the total derivative of the saddle point equation $N(\boldsymbol{\nu}^{\mathrm{sp}}, \boldsymbol{v}^{\mathrm{sp}}) = t$ with respect to N,

$$(\boldsymbol{\nu}^{\mathrm{sp}}, \boldsymbol{v}^{\mathrm{sp}}) + N \left[(\partial_{x_0^{\mathrm{sp}}} \boldsymbol{\nu}^{\mathrm{sp}}, \boldsymbol{v}^{\mathrm{sp}}) - (\boldsymbol{\nu}^{\mathrm{sp}}, \boldsymbol{w}^{\mathrm{sp}}) \right] \partial_N x_0^{\mathrm{sp}} = 0,$$

and by observing that, according to equation (67), we have

$$(\partial_{x_0^{\mathrm{sp}}} \boldsymbol{\nu}^{\mathrm{sp}}, \boldsymbol{v}^{\mathrm{sp}}) = -\sum_{k=2}^{\infty} \frac{N^{k-1}}{(k-2)!} \langle (\boldsymbol{\nu}, \boldsymbol{u}^{\mathrm{sp}})^{k-2} (\boldsymbol{\nu}, \boldsymbol{v}^{\mathrm{sp}})^2 \rangle_N^{(c)}$$
$$= -(\boldsymbol{\Sigma} \boldsymbol{v}^{\mathrm{sp}}, \boldsymbol{v}^{\mathrm{sp}}).$$

To evaluate the integral (74), we approximate $\psi(N) \simeq \psi(N^{\mathrm{sp}}) + \frac{1}{2} \partial_N^2 \psi(N^{\mathrm{sp}})(N - N^{\mathrm{sp}})^2$ and $C_N \simeq C_{N^{\mathrm{sp}}}$. The remaining Gaussian integration gives the following result:

$$\mathsf{E}(\mathcal{M}_{\boldsymbol{n}_0}^t) = \sqrt{\frac{1 + \mathrm{tr}(\boldsymbol{\Sigma} \boldsymbol{A})}{|\det(\boldsymbol{1} + \boldsymbol{\Sigma} \boldsymbol{A})|}} \frac{\mathrm{e}^{x_0^{\mathrm{sp}} t}}{\epsilon(\boldsymbol{\nu}^{\mathrm{sp}}, \boldsymbol{v}^{\mathrm{sp}})} \bigg|_{N=N^{\mathrm{sp}}}. \tag{83}$$

The matrices $\boldsymbol{\Sigma}$ and $\boldsymbol{A}$ are defined by equations (71) and (72) and their components explicitly read

$$\Sigma_{\alpha,\beta} = \Sigma_{\alpha,\beta}^{(N;2)} + \sum_{k=1}^{\infty} \frac{1}{k!} \sum_{\alpha_1 \in \mathscr{H}} \cdots \sum_{\alpha_k \in \mathscr{H}} \Sigma_{\alpha,\beta,\alpha_1,\ldots,\alpha_k}^{(N;k+2)} u_{\alpha_1}^{\mathrm{sp}} \cdots u_{\alpha_k}^{\mathrm{sp}}, \tag{84}$$

$$A_{\alpha,\beta} = \frac{v_\alpha^{\mathrm{sp}} v_\beta^{\mathrm{sp}}}{(\boldsymbol{\nu}^{\mathrm{sp}}, \boldsymbol{w}^{\mathrm{sp}})}. \tag{85}$$

Equation (83) represents our final expression for the matrix elements (14). It is valid for t large but finite with $N^{\mathrm{sp}}(t)$ determined by equation (80). It is simple to show that in the limit $t \to \infty$, equation (80) may admit a solution only if $N^{\mathrm{sp}}(t)$ grows proportionally to t. In fact, from equation (52b) for arbitrary t and N we have that

$$\nu_{V_{\min}}^{\mathrm{sp}} \frac{N+1}{t} < x_0^{\mathrm{sp}} + V_{\min} \leq \frac{N+1}{t}, \tag{86}$$

where $V_{\min}$ is the smallest value of $V \in \mathscr{V}$ such that $\nu_{V_{\min}}^{\mathrm{sp}} > 0$. Note that this value of V exists due to the properties $0 \leq \nu_{\alpha}^{\mathrm{sp}} \leq 1$ for any $\alpha \in \mathscr{V}$ and $\sum_{\alpha \in \mathscr{V}} \nu_{\alpha}^{\mathrm{sp}} = 1$. Therefore, for $N = N_{\mathrm{sp}}(t)$ all the components $u_V = -\log[(x_0^{\mathrm{sp}} + V)/\varepsilon]$ diverge when $t \to \infty$ if $\lim_{t \to \infty} N^{\mathrm{sp}}(t)/t = \infty$, whereas if $\lim_{t \to \infty} N^{\mathrm{sp}}(t)/t = 0$ the only diverging component is $u_{V_{\min}}$. In both cases, equation (80) does not have a solution for $t \to \infty$. In this limit, therefore, we must have $N^{\mathrm{sp}}(t) \sim t$. This condition, which from a physical point of view simply expresses the proportionality between the time and the length of the trajectories most contributing to the expectation, implies two important consequences. First, since the peak of the Gaussian at $N = N^{\mathrm{sp}}(t)$ moves to infinity linearly with t, whereas its width increases only as $\sqrt{t}$, see equations (81) and (82), the result (83) becomes asymptotically exact for $t \to \infty$. Second, in equation (80) we can replace $\mathbf{\Sigma}^{(N;k)}$ by their asymptotic values $\mathbf{\Sigma}^{(k)}$. In this way, equation (80) can be read as a time-independent equation that determines the quantity

$$E_{0\mathrm{B}} = - \lim_{t \to \infty} x_0^{\mathrm{sp}}|_{N = N^{\mathrm{sp}}(t)} \tag{87}$$

as a function of the asymptotic rescaled cumulants $\mathbf{\Sigma}^{(k)}$, $k \geq 1$. Comparing equations (15) and (83), we realize that this quantity is the ground-state energy of the system considered. In conclusion, for systems of hard-core bosons the ground-state energy $E_{0\mathrm{B}}$ is determined by the scalar equation

$$\sum_{k=1}^{\infty} \frac{1}{k!} \sum_{\alpha_1 \in \mathscr{H}} \cdots \sum_{\alpha_k \in \mathscr{H}} \Sigma_{\alpha_1,\dots,\alpha_k}^{(k)} u_{\alpha_1}(E_{0\mathrm{B}}) \cdots u_{\alpha_k}(E_{0\mathrm{B}}) = 0 \qquad E_{0\mathrm{B}} \leq V_{\min}, \tag{88}$$

where

$$\boldsymbol{u}^{\mathrm{T}}(E_{0\mathrm{B}}) = (\cdots - \log[(-E_{0\mathrm{B}} + V)/\epsilon] \cdots ; \cdots \log T \cdots). \tag{89}$$

The existence of a unique solution of equation (88) is ensured by the condition $E_{0\mathrm{B}} \leq V_{\min}$, which stems from equation (52b). If we truncate the series in equation (88) to the second order, we recover the Gaussian approximation of [5] (there $\mathbf{\Sigma}^{(1)}$ and $\mathbf{\Sigma}^{(2)}$ were indicated as $\overline{\boldsymbol{\nu}}$ and $\mathbf{\Sigma}$, respectively). Furthermore, as in [5], the $\hat{V} \equiv 0$ case can be solved explicitly and we get the following exact solution for the ground-state energy, $E_{0\mathrm{B}}^{(0)}$, of a non-interacting hard-core boson system:

$$E_{0\mathrm{B}}^{(0)} = -\epsilon \exp \left[\sum_{k=1}^{\infty} \frac{1}{k!} \sum_{T_1 \in \mathscr{T}} \cdots \sum_{T_k \in \mathscr{T}} \Sigma_{T_1,\dots,T_k}^{(k)} \log T_1 \cdots \log T_k \right]. \tag{90}$$

For a generic $\hat{V}$, equation (88), with the series truncated at an arbitrary finite order $k_{\max}$, can be solved numerically by the bisection method using the bounds $E_{0\mathrm{B}}^{(0)} + V_{\min} \leq E_{0\mathrm{B}} \leq V_{\min}$.

Equation (88) allows one, via the Hellmann–Feynman theorem (5), also to evaluate the expectation of any other operator in the ground state of the chosen Hamiltonian (see [5] for more details). Moreover, it is clear that the cumulants $\mathbf{\Sigma}^{(k)}$ depend only on the structure of the system Hamiltonian, not on the values of the Hamiltonian parameters. Therefore, once the $\mathbf{\Sigma}^{(k)}$ are known, all the evaluated ground-state expectations are analytical functions of the Hamiltonian parameters.

5. Numerical evaluation of the cumulants and example cases

In this section, we discuss the numerical evaluation of the cumulants. We also apply our method to some example cases and compare the ground-state energies obtained from equation (88) with those from exact numerical calculations.

In our approach, the starting point is the evaluation of the asymptotic values $\mathbf{\Sigma}^{(k)}$ of the rescaled cumulants $\mathbf{\Sigma}^{(N;k)}$. According to equation (A.7), the latter are obtained in terms of the statistical moments $\langle N_{\alpha_1} \cdots N_{\alpha_k} \rangle_N$, which are easily sampled by generating M random trajectories branching from the initial configuration $\boldsymbol{n}_0$, i.e.

$$\langle N_{\alpha_1} \cdots N_{\alpha_k} \rangle_N = \sum_{\boldsymbol{\mu}} \mathcal{P}_N(\boldsymbol{\mu}) N_{\alpha_1} \cdots N_{\alpha_k}$$

$$\simeq \frac{1}{M} \sum_{p=1}^{M} N_{\alpha_1}^{(p)} \cdots N_{\alpha_k}^{(p)}, \tag{91}$$

where $N_\alpha^{(p)}$ is the multiplicity N_α, $\alpha \in \mathcal{H}$, of the pth trajectory. The number M of trajectories must be chosen larger than a critical value $M_\varepsilon(N, k)$, which depends on the statistical precision ε required in the evaluation of the rescaled cumulants $\mathbf{\Sigma}^{(N;k)}$.

The length N of the M trajectories is chosen sufficiently large for the asymptotic behaviour of $\mathbf{\Sigma}^{(N;k)}$ to be established. This may represent a problem since the fluctuations in equation (91) grow as N^k so that $M_\varepsilon(N, k)$ becomes huge for $k > 1$. However, the evolving trajectories form a Markov chain having, see later, a finite correlation length N_c. Therefore, $\mathbf{\Sigma}^{(N;k)}$ converges exponentially to $\mathbf{\Sigma}^{(k)}$ with a characteristic length of the order of $(k + 1)N_c$, kN_c if the initial configuration $\boldsymbol{n}_0$ is taken randomly distributed according to the invariant measure of the Markov chain. As shown in the example case of figure 2, for a large class of models we have observed that the correlation length N_c exists and grows no more than linearly with the size of the system. The evaluation of the cumulants is thus feasible even for large systems.

A possible numerical limitation in the evaluation of the cumulants of large order is collecting and updating all the components of $\mathbf{\Sigma}^{(k)}$, whose number is m^k, with m the cardinality of $\mathcal{H}$, which grows with the size of the system. Basically, this kind of difficulty is related to the CPU capability of simultaneously updating many addresses of memory, not to the CPU speed, and can be reduced by vectorization tools. The difficulty can be reduced also by exploiting the invariance of the components $\Sigma_{\alpha_1,...,\alpha_k}^{(k)}$ under permutation of any pair of the α indices. In this way, only the components $\Sigma_{\alpha_1,...,\alpha_k}^{(k)}$ with $\alpha_1 \leq \alpha_2 \leq \cdots \leq \alpha_k$ are sampled according to equation (91). This introduces an error in the summation rules (60) and (61), which, on the other hand, are identically satisfied if all the components of $\mathbf{\Sigma}^{(k)}$ are sampled. However, more than a drawback this error represents an advantage, which allows one to set the critical number M_ε of
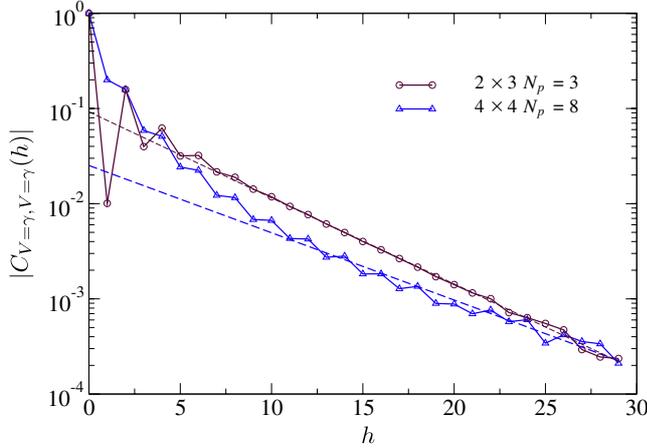
Figure 2. Absolute value of the normalized correlation function $C_{V=\gamma,V=\gamma}(h)$ as a function of the jump interval $h = h_2 - h_1$ for two different FNU hard-core boson Hubbard models. The straight dashed lines are the results of a fit in the range $10 \le h \le 29$ with a function of the form $const \times \exp(-h/N_c)$. We have $N_c = 4.80$ and $N_c = 6.14$ in the 2×3 $N_p = 3$ and 4×4 $N_p = 8$ cases, respectively. Each correlation function has been evaluated by using $M = 5 \times 10^8$ independent trajectories.

sampling trajectories in a simple way. In fact, the determination of the cumulants with a statistical precision ε implies the summation rules (60) and (61) to be satisfied with the same precision.

In the following, we report on simulations performed in the case of the first-neighbour uniform (FNU) hard-core boson Hubbard model defined by the Hamiltonian

$$\hat{H} = -\eta \sum_{(i,j)\in\Gamma} \sum_{\sigma=\uparrow\downarrow} (\hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + \hat{c}_{j\sigma}^\dagger \hat{c}_{i\sigma}) + \gamma \sum_{i\in\Lambda} \hat{c}_{i\uparrow}^\dagger \hat{c}_{i\uparrow} \hat{c}_{i\downarrow}^\dagger \hat{c}_{i\downarrow}, \tag{92}$$

where $\Gamma = \{(i,j) : i < j \in \Lambda \text{ and } i, j \text{ first neighbours}\}$. We set the reference energy ϵ to the value of the hopping parameter η. We have considered two-dimensional systems with periodic boundary conditions, $L_x \times L_y$ sites and $N_\uparrow = N_\downarrow = N_p$ particles per spin. For this model, the set $\mathscr{V}$ has elements $0, \gamma, 2\gamma, \ldots, N_p\gamma$, whereas the set $\mathscr{T}$ is the collection of the possible values of the number of active links, e.g., $\mathscr{T} = \{12, 16, 20\}$ in the case of a 2×3 system with $N_p = 3$ or $\mathscr{T} = \{8, 10, 12, 14, 16\}$ for the same system with $N_p = 2$.

To check the correlation properties mentioned before, we studied the connected correlation functions of order 2:

$$C_{\alpha,\beta}(h_2 - h_1) = \langle \chi_\alpha(\boldsymbol{n}_{h_1}) \chi_\beta(\boldsymbol{n}_{h_2}) \rangle_N^{(c)}, \tag{93}$$

where $h_2 \ge h_1$ and $\chi_\alpha(\boldsymbol{n})$ is the characteristic function taking the value 1, if $V(\boldsymbol{n}) = \alpha$ and $\alpha \in \mathscr{V}$, or $T(\boldsymbol{n}) = \alpha$ and $\alpha \in \mathscr{T}$, and 0 otherwise. The averages $\langle \cdot \rangle_N^{(c)}$ can be sampled as indicated in equation (91) by generating M independent trajectories with configurations $\boldsymbol{n}_h^{(p)}$, $h = 0, 1, \ldots, N$ and $p = 1, \ldots, M$. For N sufficiently large, the correlation functions (93) no longer depend on h_1 and h_2, only on the jump interval $h = h_2 - h_1$. In figure 2 we show the behaviour of the correlation function (normalized to 1 at $h = 0$) obtained
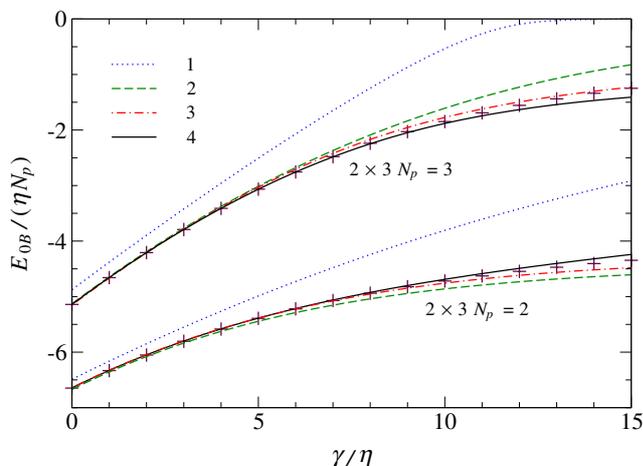
Figure 3. Ground-state energy per particle for the 2×3 FNU hard-core boson Hubbard model versus the interaction strength γ with $N_p = 2$ and 3 particles per spin. We compare the results obtained by solving equation (88) at truncation orders $k_{\max} = 1, 2, 3, 4$ (different lines) with those from exact numerical diagonalizations (+). The statistical errors associated with the cumulants, evaluated with $N = 200$ and $M = 10^7$, are negligible on this scale.

by choosing α and β equal to the potential value $V = \gamma$ for two different FNU hard-core boson Hubbard models. After an initial transient, $C_{V=\gamma,V=\gamma}(h)$ decreases as $\exp(-h/N_{\mathrm{c}})$. The measurement of the correlation length via a fitting procedure shows that N_{c} increases slowly with the size of the system. Similar results are obtained for different choices of α and β.

In figure 3 we show the behaviour of $E_{0\mathrm{B}}$ as a function of the interaction strength γ in a 2×3 lattice with $N_p = 2$ and 3, whereas in figure 4 we consider a 4×4 lattice with $N_p = 5$ and 8. In these figures, we compare the energies obtained from equation (88) by truncating the cumulant expansion at the order $k_{\max} = 1, 2, 3, 4$ with the results from exact numerical diagonalizations (figure 3) and quantum Monte Carlo simulations (figure 4). For $k_{\max} = 2$, we recover the results of [5]. As expected, we obtain better and better agreement with the exact energies as the truncation order $k_{\max}$ is increased.

The number of cumulants needed to obtain a given approximation grows as the interaction strength γ or the lattice size $|\Lambda|$ is increased. As explained in the previous sections and anticipated in [5], this behaviour is due to the form of the function $f(\boldsymbol{\mu})$ to be averaged in equation (58). In fact, $f(\boldsymbol{\mu})$ involves multiplicities $\boldsymbol{\mu}$ coupled with the potential values and with the number of active links, which, in turn, are related to γ and $|\Lambda|$. For increasing values of γ and $|\Lambda|$, $f(\boldsymbol{\mu})$ becomes more and more sensitive to the large deviations of the probability density $\mathcal{P}_N(\boldsymbol{\mu})$ and cumulants of higher and higher order must be kept in the calculation.

In figure 5, which is an enlargement of figure 3 (left panel) and figure 4 (right panel) in the small γ region of the systems at half-filling considered there, we can better appreciate the convergence of the solutions of equation (88), for increasing values of $k_{\max}$, toward the exact energies. In figures 3–5, the statistical errors associated with the measurement of the cumulants are negligible on the scales considered.
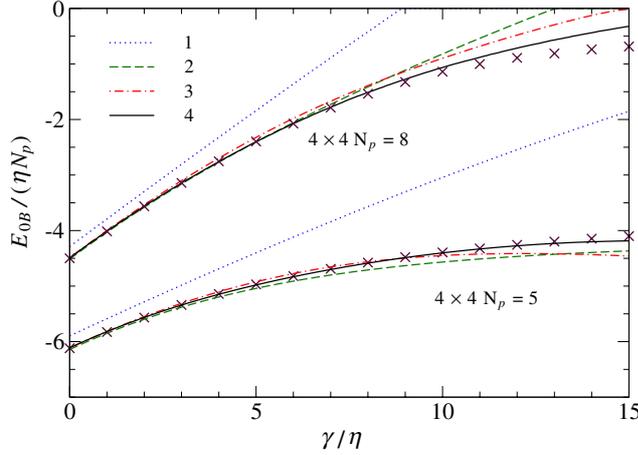
Figure 4. As figure 3, but for the 4×4 lattice with $N_p = 5$ and 8 particles per spin. We compare the results obtained by solving equation (88) at truncation orders $k_{\max} = 1, 2, 3, 4$ (different lines) with those from quantum Monte Carlo simulations ($\times$). The statistical errors associated with the cumulants, evaluated with $N = 200$ and $M = 10^7$, and with the quantum Monte Carlo results are negligible on this scale.
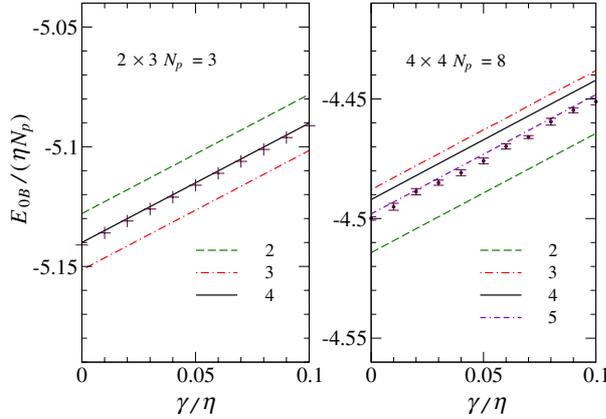
Figure 5. Enlargements of figure 3 (left panel) and figure 4 (right panel) in the small γ region of the systems at half-filling considered there. We show the results obtained by solving equation (88) at truncation orders $k_{\max} = 2, 3, 4$ (different lines, left panel) and $k_{\max} = 2, 3, 4, 5$ (different lines, right panel) in comparison with those from exact numerical diagonalizations ($+$, left panel) and quantum Monte Carlo simulations (dots with error bars, right panel). The statistical errors associated with the cumulants are negligible.

6. Conclusions

By using saddle point techniques and a cumulant expansion theorem, we have exploited an exact probabilistic representation of the quantum dynamics in a lattice to evaluate the matrix elements of the evolution operator of a system of hard-core bosons in the limit of long times. The approach yields a simple scalar equation for the ground-state energy

in terms of the asymptotic cumulants $\boldsymbol{\Sigma}^{(k)}$ of the values of the potentials, V, and of the kinetic quantities, T, assumed by the system during its long-time evolution. Since the cumulants depend only on the structure of the system Hamiltonian, once they are known, this equation provides the ground-state energy and, via the Hellmann–Feynman theorem (5), the ground-state expectation of any other operator, analytically as a function of the Hamiltonian parameters. In contrast, quantum Monte Carlo methods require, due to the unavoidable branching or reconfiguration techniques (see [7] and [11] and references therein), different simulations for different values of the parameters.

The analytical character of the present approach suggests many potential applications. Here, we briefly envisage some of them.

(i) The knowledge of the ground-state energy as a function of the Hamiltonian parameters, $E_{0\mathrm{B}} = E_{0\mathrm{B}}(\boldsymbol{\xi})$, allows in principle the determination of ground-state quenched averages, $\int f(E_{0\mathrm{B}}(\boldsymbol{\xi}))\,\mathrm{d}P_{\boldsymbol{\xi}}$, of crucial interest in the study of disordered systems. Here, $P_{\boldsymbol{\xi}}$ is a given probability density of the disorder parameters $\boldsymbol{\xi}$. Note that when the dimension of the space of the Hamiltonian parameters is larger than 1, the evaluation of the above integral by a quantum Monte Carlo approach may be a hard, if not unmanageable, numerical task.

(ii) Even though we have specialized the study to the easiest case, namely that of hard-core bosons in the absence of a magnetic field, as evidenced in section 3 and in section 4.1, our approach is general and not limited to hard-core boson systems. Fermions and bosons in a magnetic field may in principle be treated in a similar way, provided that we properly take into account also the multiplicities N_λ; see equation (18a). This possibility is of great interest since, as is well known, fermions and bosons in a magnetic field are both affected by the so-called sign (or phase) problem, which in practice inhibits the accomplishing of unbiased quantum Monte Carlo simulations.

(iii) We note that our approach is also analytical in the time parameter, t. By properly taking into account the derivatives of the cumulants with respect to the number of jumps, $\partial_N \boldsymbol{\Sigma}^{(N;k)}$, one can obtain not only the asymptotic behaviour of the matrix elements, equation (83), but also their behaviour at finite times, t, either imaginary or real. The latter possibility constitutes another chance of great interest because in general, due to the presence of oscillating terms, the real-time behaviour is also affected by a sort of sign problem and the quantum Monte Carlo simulations are reliable only for short times [7]. Of course, the complete knowledge of the time behaviour would imply that of the excited states.

(iv) Finally, we mention a different possible application of the result (88). This equation can be exploited in a Monte Carlo framework for effectively sampling the ground-state energy. Essentially, the better efficiency of this Monte Carlo method, compared with that directly deduced from equation (12), see [7] for details, follows from the fact that the stochastic times of the original probabilistic representation have been analytically integrated out, as is done in section 4.2, so that the fluctuations are necessarily reduced.

Acknowledgments

Appendix A. Proof of the cumulant summation rules

In this appendix we prove the relations (60) and (61). Due to the constraints (56), it is trivial that the statistical moments (non-connected correlation functions) of order k, $\langle \nu_{\alpha_1} \cdots \nu_{\alpha_k} \rangle_N$, $\alpha_1, \ldots, \alpha_k \in \mathscr{H}$, satisfy the following summation rules:

$$\sum_{\alpha \in \mathscr{V}} \langle \nu_\alpha \rangle_N = \sum_{\alpha \in \mathscr{T}} \langle \nu_\alpha \rangle_N = 1, \tag{A.1}$$

for $k = 1$, whereas for $k > 1$

$$\sum_{\alpha_k \in \mathscr{V}} \langle \nu_{\alpha_1} \cdots \nu_{\alpha_k} \rangle_N = \sum_{\alpha_k \in \mathscr{T}} \langle \nu_{\alpha_1} \cdots \nu_{\alpha_k} \rangle_N$$
$$= \langle \nu_{\alpha_1} \cdots \nu_{\alpha_k-1} \rangle_N. \tag{A.2}$$

Since $\langle \nu_\alpha \rangle_N^{(c)} = \langle \nu_\alpha \rangle_N$, equation (A.1) coincides with equation (60).

To demonstrate equation (61), let us introduce the short notation

$$m(I^{(k)}) = \langle \nu_{\alpha_1} \cdots \nu_{\alpha_k} \rangle_N \tag{A.3}$$

$$s(I^{(k)}) = \langle \nu_{\alpha_1} \cdots \nu_{\alpha_k} \rangle_N^{(c)}, \tag{A.4}$$

where $I^{(k)} = \{1, \ldots, k\}$ is the set of integers that appear as subscripts in $\alpha_1 \ldots \alpha_k$. More generally, for any nonempty subset I_p of $I^{(k)}$, $I_p = \{p_1, p_2, \ldots\}$, we define $m(I_p)$ and $s(I_p)$ as

$$m(I_p) = \langle \nu_{\alpha_{p_1}} \nu_{\alpha_{p_2}} \cdots \rangle_N \tag{A.5}$$

$$s(I_p) = \langle \nu_{\alpha_{p_1}} \nu_{\alpha_{p_2}} \cdots \rangle_N^{(c)}. \tag{A.6}$$

The cumulants can be defined implicitly in terms of the moments according to the relation [8]

$$m(I^{(k)}) = \sum_{\cup_p I_p = I^{(k)}} \prod_p s(I_p), \tag{A.7}$$

where the sum is extended to all the unordered decompositions of the set $I^{(k)}$ in disjoint nonempty sets I_p such that $\cup_p I_p = I^{(k)}$.

Let us proceed inductively and suppose that equations (61) hold for any value of the order k such that $2 \leq k \leq n - 1$, i.e.

$$\sum_{\alpha_k} s(I^{(k)}) = 0, \qquad 2 \leq k \leq n - 1, \tag{A.8}$$

where the sum runs either over the sets $\mathscr{V}$ or $\mathscr{T}$.

At the order n, we rewrite equation (A.7) as

$$m(I^{(n)}) = s(I^{(n)}) + \sum_{\cup_p I_p = I^{(n-1)}} \prod_p s(I_p) s(\{n\}) + \sum_{\cup_p I_p = I^{(n)}, I_p \neq I^{(n)}, I_p \neq \{n\}} \prod_p s(I_p), \tag{A.9}$$

where $\{n\}$ is the set having only the element n and $s(\{n\}) = \langle \nu_{\alpha_n} \rangle_N^{(c)}$. By summing over the index α_n, for $\alpha_n \in \mathcal{V}$ or $\alpha_n \in \mathcal{T}$, and using the relations (A.2) together with $\langle \nu_{\alpha_n} \rangle_N^{(c)} = \langle \nu_{\alpha_n} \rangle_N$, we get

$$m(I^{(n-1)}) = \sum_{\alpha_n} s(I^{(n)}) + \sum_{\cup_p I_p = I^{(n-1)}} \prod_p s(I_p) + \sum_{\cup_p I_p = I^{(n)}, \ I_p \neq I^{(n)}, \ I_p \neq \{n\}} \prod_p \sum_{\alpha_n} s(I_p). \quad \text{(A.10)}$$

According to equation (A.7), the second term in the rhs of equation (A.10) is equal to $m(I^{(n-1)})$ whereas the third term involves only sets I_p with $|I_p| \leq n-1$ so that by using the inductive hypothesis, equations (A.8), we have

$$\sum_{\alpha_n} s(I^{(n)}) = 0. \quad \text{(A.11)}$$

Finally, it is easy to verify by direct inspection that in the case $k = 2$ we have

$$\sum_{\alpha_2} s(I^{(2)}) = 0, \quad \text{(A.12)}$$

so that equation (61) is proved.

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