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Ground state of many-body lattice systems: an analytical probabilistic approach

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Abstract. On the grounds of a Feynman–Kac-type formula for Hamiltonian lattice systems, we derive analytical expressions for the matrix elements of the evolution operator. These expressions are valid at long times when a central limit theorem applies. As a remarkable result, we find that the ground-state energy as well as all the correlation functions in the ground state are determined semi-analytically by solving a simple scalar equation. Furthermore, explicit solutions of this equation are obtained in the noninteracting case.

Contents

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1. Introduction

The Feynman–Kac formula [1] provides a powerful connection between the imaginary time evolution of quantum systems in the continuum and probabilistic expectations over Wiener classical trajectories. Its extension to the case of multicomponent wavefunctions requires the introduction of a further expectation over stochastic Poisson processes [2]. The role of Poisson processes is central in the probabilistic representation of Berezin integrals over anticommuting variables and, in general, of the time evolution of discrete systems [3]. In the simplified formulation [4], it is shown that the real or the imaginary time dynamics of systems described by a finite Hamiltonian matrix, representing bosonic or fermionic degrees of freedom, is expressed in terms of the evolution of a proper collection of independent Poisson processes. For a lattice system, the Poisson processes are associated with the links of the lattice and their jump rates can be arbitrary. In [4], it is demonstrated that when the rates of the Poisson processes are chosen equal to the hopping coefficients of the system, the probabilistic representation leads to an optimal algorithm which coincides with the Green function quantum Monte Carlo (QMC) method [5]–[7] in the limit when the latter becomes exact [8].

In the present paper, we exploit the probabilistic representation [4] to derive analytical expressions for the matrix elements of the evolution operator in the long time limit. Our approach is based on a series expansion of the probabilistic expectation in terms of conditional expectations with a fixed number N of jumps of the Poisson processes. This resembles the expansion of the grand canonical partition function in statistical mechanics in terms of canonical averages with a fixed number of particles. By integrating out the N stochastic jump times, we show that the conditional expectations become averages of functions, which depend only on the multiplicities N_V and N_A of the values assumed by the potential and hopping energies, respectively, of the configurations visited by the system. According to a central limit theorem, at large values of N, i.e. long times, the rescaled multiplicities $N_V/\sqrt{N}$ and $N_A/\sqrt{N}$ become Gaussian-distributed and the corresponding averages can be evaluated analytically. The parameters of the Gaussian probability density do not depend on the Hamiltonian parameters and are easily determined statistically. Finally, the series of the conditional expectations can be re-summed with a saddle-point method. As a remarkable result, we find that the ground-state energy is semi-analytically determined by solving a simple scalar equation. Once this equation is solved the quantum expectation in the ground state for other operators can be determined analytically by using the Hellman–Feynman theorem. The result is valid for boson or fermion systems. As regards fermions, the well-known sign problem [8]–[13] is avoided by introducing an approximation related to the exact counting of the positive and negative contributions in the noninteracting case.

The paper is organized as follows. In section 2, we review the probabilistic representation of quantum dynamics for a generalized Hubbard Hamiltonian. In section 3, we decompose the expectation in canonical averages of weights, which are calculated analytically. The canonical averages are evaluated at long times via a central limit theorem in section 4. The equation for the ground-state energy is discussed in section 4.1 for hard-core bosons and in section 4.2 for fermions. In section 5, we show how to calculate ground-state correlation functions within our approach. Finally, in section 6, we show some example cases and compare with the results of exact numerical calculations. General features of our approach are summarized and discussed in section 7.

2. Exact probabilistic representation of lattice dynamics

We illustrate our approach for imaginary time dynamics for a system of hard-core bosons or fermions described by a generalized Hubbard Hamiltonian

$$H = -\sum_{i\neq j\in\Lambda}\sum_{\sigma=\uparrow\downarrow}\eta_{ij}c^{\dagger}_{i\sigma}c_{j\sigma} + \sum_{i\in\Lambda}\gamma_i c^{\dagger}_{i\uparrow}c_{i\uparrow}c^{\dagger}_{i\downarrow}c_{i\downarrow} + \sum_{i\in\Lambda}\sum_{\sigma=\uparrow\downarrow}\delta_{i\sigma}c^{\dagger}_{i\sigma}c_{i\sigma}, \tag{1}$$

where $\Lambda \subset Z^d$ is a finite d-dimensional lattice with $|\Lambda|$ sites and $c_{i\sigma}$ the commuting or anticommuting destruction operators at site i and spin index σ with the property $c^2_{i\sigma} = 0$. We are interested in evaluating the matrix elements $\langle \boldsymbol{n}|\mathrm{e}^{-Ht}|\boldsymbol{n}_0\rangle$, where $\boldsymbol{n} = (n_{1\uparrow}, n_{1\downarrow}, \ldots, n_{|\Lambda|\uparrow}, n_{|\Lambda|\downarrow})$ are the lattice occupation numbers taking the values 0 or 1. The total number of particles is $N_\sigma = \sum_{i\in\Lambda} n_{i\sigma}$ for $\sigma = \uparrow\downarrow$. In the following, we shall use the mod 2 addition $n \oplus n' = (n + n') \bmod 2$.

Let Γ be the set of system links, i.e. the unordered pairs (i, j) with $i, j \in \Lambda$ such that $\eta_{ij} \neq 0$. For simplicity, we will start by assuming $\eta_{ij} = \epsilon$ if i and j are first neighbours and $\eta_{ij} = 0$ otherwise. We will also assume $\gamma_i = \gamma$ and $\delta_i = 0$. We shall call such a model the first neighbour uniform (FNU) model. For a d-dimensional lattice the number of links per spin component is $|\Gamma| = d|\Lambda|$. Let us introduce

$$\lambda_{ij\sigma}(\boldsymbol{n}) = \langle \boldsymbol{n} \oplus \mathbf{1}_{i\sigma} \oplus \mathbf{1}_{j\sigma}|c^{\dagger}_{i\sigma}c_{j\sigma} + c^{\dagger}_{j\sigma}c_{i\sigma}|\boldsymbol{n}\rangle, \tag{2}$$

$$V(\boldsymbol{n}) = \langle \boldsymbol{n}|H|\boldsymbol{n}\rangle, \tag{3}$$

where $\mathbf{1}_{i\sigma} = (0, \ldots, 0, 1_{i\sigma}, 0, \ldots, 0)$, and let $\{N^t_{ij\sigma}\}$, $(i, j) \in \Gamma$, be a family of $2|\Gamma|$ independent Poisson processes with jump rate ρ. At each jump of the process $N^t_{ij\sigma}$, if $\lambda_{ij\sigma} \neq 0$ a particle moves from site i to site j or vice versa, whereas the lattice configuration $\boldsymbol{n}$ remains unchanged if $\lambda_{ij\sigma} = 0$. The total number of jumps at time t is $N_t = \sum_{(i,j)\in\Gamma,\sigma=\uparrow\downarrow} N^t_{ij\sigma}$. By ordering the jumps according to the times s_k, $k = 1, \ldots, N_t$, which take place in the interval $[0, t)$, we define a trajectory as the Markov chain $\boldsymbol{n}_1, \boldsymbol{n}_2, \ldots, \boldsymbol{n}_{N_t}$ generated from the initial configuration $\boldsymbol{n}_0$. Let us call $\lambda_1, \lambda_2, \ldots, \lambda_{N_t}$ and $V_1, V_2, \ldots, V_{N_t}$ the values of the matrix elements (2) and (3) occurring along the trajectory. As proved in [4], the following representation holds:

$$\langle \boldsymbol{n}|\mathrm{e}^{-Ht}|\boldsymbol{n}_0\rangle = \mathsf{E}(\delta_{\boldsymbol{n},\boldsymbol{n}_{N_t}}\mathcal{M}^t), \tag{4}$$

where the stochastic functional $\mathcal{M}^t$ is defined by

$$\mathcal{M}^t = \mathrm{e}^{2|\Gamma|\rho t}\left(\prod_{k=1}^{N_t}\frac{\epsilon}{\rho}\lambda_k \mathrm{e}^{-V_{k-1}(s_k - s_{k-1})}\right)\mathrm{e}^{-V_{N_t}(t-s_{N_t})} \tag{5}$$

if $N_t > 0$ and $\mathcal{M}^t = \mathrm{e}^{2|\Gamma|\rho t}\mathrm{e}^{-V_0 t}$ if $N_t = 0$. Here $V_0 = V(\boldsymbol{n}_0)$ and $s_0 = 0$.

Several quantities can be obtained from the matrix elements (4). The ground-state energy is given by

$$E_0 = \lim_{t\to\infty}\frac{-\sum_{\boldsymbol{n}}\partial_t\langle \boldsymbol{n}|\mathrm{e}^{-Ht}|\boldsymbol{n}_0\rangle}{\sum_{\boldsymbol{n}}\langle \boldsymbol{n}|\mathrm{e}^{-Ht}|\boldsymbol{n}_0\rangle} = \lim_{t\to\infty}\frac{-\partial_t\mathsf{E}(\mathcal{M}^t)}{\mathsf{E}(\mathcal{M}^t)}. \tag{6}$$

3. Canonical decomposition of expectation

To evaluate (6), we decompose the expectation $\mathsf{E}(\mathcal{M}^t)$ as a series of conditional expectations with a fixed number of jumps (canonical averages)

$$\begin{aligned}\mathsf{E}(\mathcal{M}^t) &= \sum_{N=0}^{\infty} \mathsf{E}(\mathcal{M}^t | N_t = N) \\ &= \sum_{N=0}^{\infty} \sum_{r\in\Omega_N} \mathcal{S}_N^{(r)} \mathcal{W}_N^{(r)}(t), \end{aligned} \tag{7}$$

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

$$\mathcal{S}_N^{(r)} = \lambda_1^{(r)} \lambda_2^{(r)} \dots \lambda_N^{(r)}, \tag{8}$$

$$\mathcal{W}_N^{(r)}(t) = \epsilon^N \int_0^t \mathrm{d}s_1 \int_{s_1}^t \mathrm{d}s_2 \dots \int_{s_{N-1}}^t \mathrm{d}s_N \, \mathrm{e}^{-V_0 s_1 - V_1^{(r)}(s_2 - s_1) - \dots - V_N^{(r)}(t - s_N)}. \tag{9}$$

The weights (9) are obtained on multiplying (5) by the infinitesimal probability $\mathrm{e}^{-2|\Gamma|\rho t} \rho^N \mathrm{d}s_1 \mathrm{d}s_2 \dots \mathrm{d}s_N$ to have N jumps and integrating over the jump times.

A link ij with spin σ is called active if $\lambda_{ij\sigma} \neq 0$. From (8), it is clear that only trajectories formed by a sequence of active links contribute to (7). Hereafter, we restrict Ω_N to be the set of these effective trajectories with N jumps. The sum over the set Ω_N in (7) can be rewritten as an average $\langle\cdot\rangle$ over the trajectories with N jumps generated by extracting with uniform probability one of the active links available at the configurations $\boldsymbol{n}_0, \boldsymbol{n}_1, \dots, \boldsymbol{n}_{N-1}$. If $A_k = \sum_{(i,j)\in\Gamma, \sigma=\uparrow\downarrow} |\lambda_{ij\sigma}(\boldsymbol{n}_k)|$ is the number of active links in the configuration $\boldsymbol{n}_k$, the probability associated with the trajectory r is $p_N^{(r)} = \prod_{k=0}^{N-1} 1/A_k^{(r)}$ and we have

$$\begin{aligned}\sum_{r\in\Omega_N} \mathcal{S}_N^{(r)} \mathcal{W}_N^{(r)}(t) &= \sum_{r\in\Omega_N} p_N^{(r)} \mathcal{S}_N^{(r)} \mathcal{W}_N^{(r)}(t) \prod_{k=0}^{N-1} A_k^{(r)} \\ &= \left\langle \mathcal{S}_N \mathcal{W}_N(t) \prod_{k=0}^{N-1} A_k \right\rangle. \end{aligned} \tag{10}$$

Note that $\prod_{k=0}^{N-1} A_k = \prod_A A^{N_A}$ depends only on the multiplicities N_A of the values A assumed by the number of active links; these multiplicities are normalized to N, i.e. $\sum_A N_A = N$. For the FNU model, the possible values of A depend on the number of particles and we have the bound $A \leqslant \min(2d(N_\uparrow + N_\downarrow), 2|\Gamma|)$.

For a generic trajectory, weights (9) satisfy the recursive differential equation

$$\frac{\mathrm{d}\mathcal{W}_N(t)}{\mathrm{d}t} = \mathcal{W}_{N-1}(t) - V_N \mathcal{W}_N(t), \tag{11}$$

where $\mathcal{W}_{-1}(t) = 0$. In terms of the Laplace transform $\widetilde{\mathcal{W}}_N(z) = \int_0^\infty \mathrm{d}t \, \mathrm{e}^{-zt} \mathcal{W}_N(t)$ we get

$$\widetilde{\mathcal{W}}_N(z) = \epsilon^N \prod_{k=0}^{N} \frac{1}{z + V_k} = \epsilon^N \prod_V \frac{1}{(z+V)^{N_V}}. \tag{12}$$

In (12) we see that the weights depend only on the multiplicities N_V of the values V assumed by the potential; these multiplicities are normalized to $N+1$, i.e. $\sum_V N_V = N+1$. For model (1), the possible values assumed by V are $V = 0, \gamma, 2\gamma, \ldots, N_p\gamma$, where $N_p = \min(N_\uparrow, N_\downarrow)$.

For an assigned set of multiplicities of the potential, the antitransform of (12) can be evaluated with the residue method. In this way one obtains an exact recursive expression of $\mathcal{W}_N(t)$ which, however, for large N must be evaluated numerically with multi-precision algebra. On the other hand, for N large, a complex saddle-point method can be used, which provides the following asymptotically exact explicit expression:

$$\mathcal{W}_N(t) = \frac{\mathrm{e}^{x_0 t - \sum_V N_V \log[(x_0+V)/\epsilon]}}{\sqrt{2\pi \sum_V (\epsilon^2 N_V/(x_0+V)^2)}}, \tag{13}$$

where x_0 is the solution of the equation

$$\sum_V \frac{N_V}{x_0 + V} = t. \tag{14}$$

Note that in the case $\gamma = 0$, equation (13) reduces to Stirling's approximation of the exact value $\mathcal{W}_N(t) = \epsilon^N t^N / N!$.

4. Canonical averages via a central limit theorem

As evident from the explicit expression given in the case $\gamma = 0$, the weights $\mathcal{W}_N(t)$ have a maximum at some N, which increases by increasing t. This remains true also in the general case, as shown in the following. Therefore, in the long time limit, the most important contributions to the expansion (7) of the expectation $\mathsf{E}(\mathcal{M}^t)$ come from larger and larger values of N. In this section, we will evaluate the canonical averages (10) analytically for N large by using the asymptotic behaviour of the stochastic variables N_V and N_A. In the following, we will indicate by m_V and m_A the number of different values assumed by the variables V and A, respectively. In this limit, we will not distinguish the different normalizations, $N+1$ and N, of N_V and N_A, respectively. For clarity, we consider separately the hard-core boson and fermion cases.

4.1. Hard-core bosons

In this case, we have $\mathcal{S}_N = 1$ and the canonical averages (10) are averages of a function, which depends only on the multiplicities, N_V and N_A (besides a parametric dependence on time). In terms of the corresponding frequencies, $\nu_V = N_V/N$ and $\nu_A = N_A/N$, which for N large become continuously distributed in the range [0, 1] with the constraints

$$\sum_V \nu_V = \sum_A \nu_A = 1, \tag{15}$$

equation (10) can be rewritten as

$$\left\langle \mathcal{W}_N(t) \prod_{k=0}^{N-1} A_k \right\rangle = \int \mathrm{d}\boldsymbol{\nu}\, \mathcal{P}_N(\boldsymbol{\nu}) g_N(t; \boldsymbol{\nu}), \tag{16}$$

$$g_N(t;\boldsymbol{\nu}) = \frac{\mathrm{e}^{x_0 t + N(\boldsymbol{\nu},\boldsymbol{u})}}{\sqrt{2\pi N \sum_V (\epsilon^2 \nu_V/(x_0+V)^2)}}, \tag{17}$$

where $\boldsymbol{\nu}$ and $\boldsymbol{u}$ are vectors with $m = m_V + m_A$ components defined as $\boldsymbol{\nu}^{\mathrm{T}} = (\ldots \nu_V \ldots; \ldots \nu_A \ldots)$ and $\boldsymbol{u}^{\mathrm{T}} = (\ldots -\log[(x_0+V)/\epsilon]\ldots; \ldots \log A \ldots)$, respectively. Note that $\boldsymbol{u}$ depends on $\boldsymbol{\nu}$ through $x_0 = x_0(\boldsymbol{\nu})$.

The probability density $\mathcal{P}_N(\boldsymbol{\nu})$ is given by the fraction of trajectories branching from the initial configuration $\boldsymbol{n}_0$ and having after N jumps multiplicities $N_V = \nu_V N$ and $N_A = \nu_A N$. For N large, it can be approximated in the following way. We rewrite the multiplicities as $N_V = \sum_{k=0}^{N} \chi_V(\boldsymbol{n}_k)$ and $N_A = \sum_{k=1}^{N} \chi_A(\boldsymbol{n}_{k-1})$, where $\chi_V(\boldsymbol{n}) = 1$ if $V(\boldsymbol{n}) = V$ and $\chi_V(\boldsymbol{n}) = 0$ otherwise, and similarly for χ_A. Since the configurations $\boldsymbol{n}_k$ form a Markov chain with finite-state space, a central limit theorem applies to each rescaled sum $N_V/\sqrt{N}$ or $N_A/\sqrt{N}$ [14]. However, due to the constraints (15), the joint probability for these m rescaled sums is not Gaussian. Given an arbitrary set of $m_V - 1$ V-like components and $m_A - 1$ A-like components, the joint probability density is the product of a Gaussian density for this set of variables and two delta functions, which take into account the constraints (15). For the frequencies $\boldsymbol{\nu}$, therefore, we have

$$\mathcal{P}_N(\boldsymbol{\nu}) = \mathcal{F}_N(\hat{\boldsymbol{\nu}})\delta\Big(\sum_V \nu_V - 1\Big)\delta\Big(\sum_A \nu_A - 1\Big), \tag{18}$$

where $\mathcal{F}_N(\hat{\boldsymbol{\nu}})$ is the normal density defined in terms of the vector $\hat{\boldsymbol{\nu}}$ having the $m-2$ chosen components of $\boldsymbol{\nu}$

$$\mathcal{F}_N(\hat{\boldsymbol{\nu}}) = \sqrt{\frac{N^{m-2}|\det \hat{\boldsymbol{\Sigma}}^{-1}|}{(2\pi)^{m-2}}}\mathrm{e}^{-(N/2)(\hat{\boldsymbol{\Sigma}}^{-1}(\hat{\boldsymbol{\nu}}-\hat{\overline{\boldsymbol{\nu}}}),(\hat{\boldsymbol{\nu}}-\hat{\overline{\boldsymbol{\nu}}}))}. \tag{19}$$

Here $\hat{\overline{\boldsymbol{\nu}}}$ and $\hat{\boldsymbol{\Sigma}}N^{-1}$ are the $(m-2)$-component subvector and submatrix, respectively, of the mean value, $\overline{\boldsymbol{\nu}}$, and the covariance matrix, $\boldsymbol{\Sigma}N^{-1}$, of $\boldsymbol{\nu}$. As discussed in section 6, the quantities $\overline{\boldsymbol{\nu}}$ and $\boldsymbol{\Sigma}$ are easily measured by sampling over trajectories with a large number of jumps.

By using (18), the m-dimensional integral, which appears in (16), can be performed by the saddle-point method. Note that this integration method is asymptotically exact for N large. Due to the constraints (15), $\overline{\boldsymbol{\nu}}$ satisfies the property $\sum_V \overline{\nu}_V = \sum_A \overline{\nu}_A = 1$, whereas rows and columns of the VV, VA, AV and AA blocks of $\boldsymbol{\Sigma}$ are normalized to zero. By using these properties, in terms of $\overline{\boldsymbol{\nu}}$ and $\boldsymbol{\Sigma}$, we get

$$\left\langle \mathcal{W}_N(t)\prod_{k=0}^{N-1} A_k \right\rangle = \left.\frac{\mathrm{e}^{x_0 t + N[(\overline{\boldsymbol{\nu}},\boldsymbol{u})+\frac{1}{2}(\boldsymbol{\Sigma}\boldsymbol{u},\boldsymbol{u})]}}{\sqrt{2\pi N \sum_V (\epsilon^2 \nu_V/(x_0+V)^2)}}\right|_{\boldsymbol{\nu}=\boldsymbol{\nu}^{\mathrm{sp}}}, \tag{20}$$

where $\boldsymbol{\nu}^{\mathrm{sp}}$ is the saddle-point frequency defined by the equation

$$\boldsymbol{\nu}^{\mathrm{sp}} = \overline{\boldsymbol{\nu}} + \boldsymbol{\Sigma}\boldsymbol{u}(\boldsymbol{\nu}^{\mathrm{sp}}). \tag{21}$$

To evaluate the expectation value $\mathsf{E}(\mathcal{M}^t)$, we need to sum the series (7). This can be done with a further saddle-point integration. According to equation (20), the terms of this series are

exponentially peaked at $N = N^{\mathrm{sp}}$, where N^{sp} satisfies

$$\left[\{t - N[(\overline{\boldsymbol{v}}, \boldsymbol{v}) + (\boldsymbol{\Sigma u}, \boldsymbol{v})]\}\frac{\partial x_0}{\partial N} + (\overline{\boldsymbol{v}}, \boldsymbol{u}) + \frac{1}{2}(\boldsymbol{\Sigma u}, \boldsymbol{u})\right]_{\boldsymbol{v}=\boldsymbol{v}^{\mathrm{sp}}, N=N^{\mathrm{sp}}} = 0, \tag{22}$$

with $\boldsymbol{v}^{\mathrm{T}} = (\ldots (x_0 + V)^{-1} \ldots; \ldots 0 \ldots)$. We observe that, according to equations (14) and (21), the term $\{t - N[(\overline{\boldsymbol{v}}\boldsymbol{v}, \boldsymbol{v}) + (\boldsymbol{\Sigma u}, \boldsymbol{v})]\}$ vanishes for $\boldsymbol{v} = \boldsymbol{v}^{\mathrm{sp}}$ so that the above condition reduces to

$$\left[(\overline{\boldsymbol{v}}, \boldsymbol{u}) + \frac{1}{2}(\boldsymbol{\Sigma u}, \boldsymbol{u})\right]_{\boldsymbol{v}=\boldsymbol{v}^{\mathrm{sp}}, N=N^{\mathrm{sp}}} = 0. \tag{23}$$

Equation (23) is a time-independent equation, which determines $x_0|_{\boldsymbol{v}=\boldsymbol{v}^{\mathrm{sp}}, N=N^{\mathrm{sp}}}$ as a function of $\overline{\boldsymbol{v}}$ and $\boldsymbol{\Sigma}$. According to equation (14), this means that for $\boldsymbol{v} = \boldsymbol{v}^{\mathrm{sp}}$, the quantity N^{sp} increases linearly with time so that $x_0|_{\boldsymbol{v}=\boldsymbol{v}^{\mathrm{sp}}, N=N^{\mathrm{sp}}}$ becomes independent of time. In conclusion, a saddle-point integration with respect to N of the series (7) provides

$$\mathsf{E}(\mathcal{M}^t) = \left.\frac{\mathrm{e}^{x_0 t}}{\sum_V \epsilon \nu_V/(x_0 + V)}\right|_{\boldsymbol{v}=\boldsymbol{v}^{\mathrm{sp}}, N=N^{\mathrm{sp}}}. \tag{24}$$

By taking the time derivative of this expectation and using (6), we obtain that the ground-state energy of the hard-core boson system is

$$E_{0B} = -x_0|_{\boldsymbol{v}=\boldsymbol{v}^{\mathrm{sp}}, N=N^{\mathrm{sp}}}. \tag{25}$$

Equation (23) is, therefore, the equation for the ground-state energy. It defines E_{0B} in terms of $\overline{\boldsymbol{v}}$ and $\boldsymbol{\Sigma}$ and explicitly reads

$$\begin{aligned} 0 = & -\sum_V \overline{\nu}_V \log\left(\frac{-E_{0B} + V}{\epsilon}\right) + \sum_A \overline{\nu}_A \log(A) \\ & + \frac{1}{2}\sum_{V,V'} \Sigma_{V,V'} \log\left(\frac{-E_{0B} + V}{\epsilon}\right) \log\left(\frac{-E_{0B} + V'}{\epsilon}\right) \\ & - \sum_{V,A} \Sigma_{V,A} \log\left(\frac{-E_{0B} + V}{\epsilon}\right) \log(A) \\ & + \frac{1}{2}\sum_{A,A'} \Sigma_{A,A'} \log(A) \log(A'). \end{aligned} \tag{26}$$

In the case $\gamma = 0$, the ground-state energy $E_{0B}^{(0)}$ can be solved explicitly and one has

$$E_{0B}^{(0)} = -\epsilon \exp\left[\sum_A \overline{\nu}_A \log(A) + \frac{1}{2}\sum_{A,A'} \Sigma_{A,A'} \log(A) \log(A')\right]. \tag{27}$$

Note that equation (27) is a nontrivial formula for the ground state of a system of bosons interacting via a hard-core potential. With the above expression equation (26) can be written

more compactly as

$$\log\left(\frac{-E_{0B}^{(0)}}{\epsilon}\right) = \sum_V \overline{\nu}_V \log\left(\frac{-E_{0B}+V}{\epsilon}\right) - \frac{1}{2}\sum_{V,V'} \Sigma_{V,V'} \log\left(\frac{-E_{0B}+V}{\epsilon}\right)\log\left(\frac{-E_{0B}+V'}{\epsilon}\right) + \sum_{V,A} \Sigma_{V,A} \log\left(\frac{-E_{0B}+V}{\epsilon}\right)\log(A). \tag{28}$$

By using the bounds $E_{0B}^{(0)} < E_{0B} < 0$, the scalar equation (28) can be easily solved with the bisection method.

The generalization of the above results to Hubbard Hamiltonians (1) with arbitrary parameters $\boldsymbol{\eta}, \boldsymbol{\gamma}, \boldsymbol{\delta}$ is straightforward. Equations (20)–(25) remain formally unchanged, however, the vectors $\overline{\boldsymbol{\nu}}, \boldsymbol{u}, \boldsymbol{v}$ and the covariance matrix $\boldsymbol{\Sigma}$ are modified to take into account all the possible values of the generalized potential V corresponding to the operator $\sum_{i\in\Lambda} \gamma_i c_{i\uparrow}^\dagger c_{i\uparrow} c_{i\downarrow}^\dagger c_{i\downarrow} + \sum_{i\in\Lambda}\sum_{\sigma=\uparrow\downarrow} \delta_{i\sigma} c_{i\sigma}^\dagger c_{i\sigma}$ and all the possible values of the generalized kinetic quantities $T = A\eta/\epsilon$, where now ϵ is a unity of energy and η/ϵ is the dimensionless hopping value corresponding to the current jumping link. In fact, the generalization of equation (10) consists in replacing $\prod_{k=0}^{N-1} A_k$ with $\prod_{k=0}^{N-1}(A_k\eta_k/\epsilon)$. Explicitly, now the vectors $\overline{\boldsymbol{\nu}}$ and $\boldsymbol{u}$ are

$$\begin{aligned} \overline{\boldsymbol{\nu}}^{\mathrm{T}} &= (\ldots \overline{\nu}_V \ldots; \ldots \overline{\nu}_T \ldots), \\ \boldsymbol{u}^{\mathrm{T}} &= (\ldots -\log[(x_0+V)/\epsilon] \ldots; \ldots \log T \ldots), \end{aligned} \tag{29}$$

and the generalized ground-state energy $E_{0B}^{(0)}$ corresponding to $\boldsymbol{\gamma} = \boldsymbol{\delta} = \mathbf{0}$ reads

$$E_{0B}^{(0)} = -\epsilon \exp\left[\sum_T \overline{\nu}_T \log(T) + \frac{1}{2}\sum_{T,T'} \Sigma_{T,T'} \log(T)\log(T')\right]. \tag{30}$$

Similar considerations hold for Hamiltonians with arbitrary potential operators.

4.2. Fermions

In this case, we have $\mathcal{S}_N = \pm 1$ and the canonical averages (10) are averages of a function, which depends not only on the multiplicities, N_V and N_A but also on N_-, the sign multiplicity related to $\mathcal{S}_N$ by $\mathcal{S}_N = (-1)^{N_-}$. The approach developed for hard-core bosons can be extended also to fermions by including this further multiplicity N_-. We will report on this procedure elsewhere. In the present paper, we introduce an approximation which allows to reduce the calculation of the fermion ground-state energy to that of an effectively modified hard-core boson system. This approximation is motivated by the observation that the correlations between N_- and N_V are smaller than those between N_- and N_A.

Let us consider again the FNU model. To evaluate (10) for a fermion system, we introduce the average weighted sign s_N after N jumps

$$s_N = \frac{\langle \mathcal{S}_N \mathcal{W}_N(t) \prod_{k=0}^{N-1} A_k \rangle}{\left\langle \mathcal{W}_N(t) \prod_{k=0}^{N-1} A_k \right\rangle}. \tag{31}$$

The quantity s_N is a function of the interaction strength. For $\gamma = 0$ it can be evaluated in the following way. Expanding $\sum_{\boldsymbol{n}} \langle \boldsymbol{n}| \, \mathrm{e}^{-Ht} |\boldsymbol{n}_0\rangle$ in powers of t and comparing with the expansion (7), for $\gamma = 0$ and N large, we obtain for hard-core bosons and fermions, respectively,

$$\left\langle \prod_{k=0}^{N-1} A_k \right\rangle = c_{0B}(\boldsymbol{n}_0)(-E_{0B}^{(0)}/\epsilon)^N, \tag{32}$$

$$\left\langle \mathcal{S}_N \prod_{k=0}^{N-1} A_k \right\rangle = c_{0F}(\boldsymbol{n}_0)(-E_{0F}^{(0)}/\epsilon)^N, \tag{33}$$

where $c_{0B}(\boldsymbol{n}_0)$ and $c_{0F}(\boldsymbol{n}_0)$ are coefficients related to the initial configuration $\boldsymbol{n}_0$ and $E_{0B}^{(0)}$ and $E_{0F}^{(0)}$ are the $\gamma = 0$ ground-state energies. The average weighted sign after N jumps for $\gamma = 0$ is then given by

$$s_N = \frac{c_{0F}(\boldsymbol{n}_0)}{c_{0B}(\boldsymbol{n}_0)} \mathrm{e}^{N \log(E_{0F}^{(0)}/E_{0B}^{(0)})}. \tag{34}$$

For fermions the noninteracting energy, $E_{0F}^{(0)}$, is known exactly, whereas for hard-core bosons $E_{0B}^{(0)}$ can be computed with Monte Carlo simulations or analytically as shown above. In general, $E_{0F}^{(0)}/E_{0B}^{(0)} < 1$ so that s_N vanishes exponentially for N large.

Approximating s_N with its value (34) at $\gamma = 0$ removes effectively the negative signs in the expectation $\mathsf{E}(\mathcal{M}^t)$. Therefore, this can be evaluated as for hard-core bosons with the same Gaussian probability density. In particular, the saddle-point condition for $N = N^{\mathrm{sp}}$ now becomes

$$\left[(\bar{\boldsymbol{v}}, \boldsymbol{u}) + \frac{1}{2}(\boldsymbol{\Sigma u}, \boldsymbol{u}) + \log \frac{E_{0F}^{(0)}}{E_{0B}^{(0)}} \right]_{\boldsymbol{v}=\boldsymbol{v}^{\mathrm{sp}}, N=N^{\mathrm{sp}}} = 0, \tag{35}$$

which is a time-independent equation determining $x_0|_{\boldsymbol{v}=\boldsymbol{v}^{\mathrm{sp}}, N=N^{\mathrm{sp}}}$ in the fermion case. Finally, as in the hard-core boson case, one finds that

$$E_{0F} = -x_0|_{\boldsymbol{v}=\boldsymbol{v}^{\mathrm{sp}}, N=N^{\mathrm{sp}}}, \tag{36}$$

and equation (35) becomes equal to equation (28) with E_{0B} and $E_{0B}^{(0)}$ substituted by E_{0F} and $E_{0F}^{(0)}$, respectively. However, in this case we do not have the analogue of equation (27) and $E_{0F}^{(0)}$ must be provided by an independent calculation, i.e. by exact diagonalization of the separable many-particle Hilbert space.

5. Ground-state correlation functions

The equation obtained in the previous section for the determination of the ground-state energy depends on the parameters of the Hamiltonian only explicitly through the values of the generalized potentials V and of the kinetic quantities T. In fact, the statistical moments $\bar{\boldsymbol{v}}$ and $\boldsymbol{\Sigma}$ are determined by the structure of the Hamiltonian not by the values of the Hamiltonian parameters. Therefore, we are able to evaluate the derivatives of the ground-state energy with respect to any parameter

ξ of the Hamiltonian $H(\xi)$. This allows the determination of arbitrary ground-state correlation functions via the Hellman–Feynman theorem

$$\frac{\langle E_0(\xi)|\partial_\xi H(\xi)|E_0(\xi)\rangle}{\langle E_0(\xi)|E_0(\xi)\rangle} = \partial_\xi E_0(\xi), \tag{37}$$

where $E_0(\xi)$ is the ground-state energy of $H(\xi)$. Hereafter, we assume a normalized ground state, $\langle E_0(\xi)|E_0(\xi)\rangle = 1$.

Suppose that we want to evaluate the quantum expectation of an operator O in the ground state of the Hamiltonian H. We have two possibilities.

(i) The operator O is a term of the Hamiltonian itself, e.g. $O = c^\dagger_{i\sigma}c_{j\sigma}$, with $i \neq j$, $O = c^\dagger_{i\uparrow}c_{i\uparrow}c^\dagger_{i\downarrow}c_{i\downarrow}$ or $O = c^\dagger_{i\sigma}c_{i\sigma}$ if H is the generalized Hamiltonian (1). In this case, by using equation (37) for hard-core bosons, we have

$$\langle E_{0B}(\boldsymbol{\eta},\boldsymbol{\gamma},\boldsymbol{\delta})|c^\dagger_{i\sigma}c_{j\sigma}|E_{0B}(\boldsymbol{\eta},\boldsymbol{\gamma},\boldsymbol{\delta})\rangle = -\partial_{\eta_{ij}}E_{0B}(\boldsymbol{\eta},\boldsymbol{\gamma},\boldsymbol{\delta})$$

$$= \frac{\sum_T (\nu^{\rm sp}_T/T)\partial_{\eta_{ij}}T}{\sum_V \nu^{\rm sp}_V/(-E_{0B}(\boldsymbol{\eta},\boldsymbol{\gamma},\boldsymbol{\delta})+V)}, \qquad i \neq j, \tag{38}$$

$$\langle E_{0B}(\boldsymbol{\eta},\boldsymbol{\gamma},\boldsymbol{\delta})|c^\dagger_{i\uparrow}c_{i\uparrow}c^\dagger_{i\downarrow}c_{i\downarrow}|E_{0B}(\boldsymbol{\eta},\boldsymbol{\gamma},\boldsymbol{\delta})\rangle = \partial_{\gamma_i}E_{0B}(\boldsymbol{\eta},\boldsymbol{\gamma},\boldsymbol{\delta})$$

$$= \frac{\sum_V (\nu^{\rm sp}_V/(-E_{0B}(\boldsymbol{\eta},\boldsymbol{\gamma},\boldsymbol{\delta})+V))\partial_{\gamma_i}V}{\sum_V \nu^{\rm sp}_V/(-E_{0B}(\boldsymbol{\eta},\boldsymbol{\gamma},\boldsymbol{\delta})+V)}, \tag{39}$$

$$\langle E_{0B}(\boldsymbol{\eta},\boldsymbol{\gamma},\boldsymbol{\delta})|c^\dagger_{i\sigma}c_{i\sigma}|E_{0B}(\boldsymbol{\eta},\boldsymbol{\gamma},\boldsymbol{\delta})\rangle = \partial_{\delta_{i\sigma}}E_{0B}(\boldsymbol{\eta},\boldsymbol{\gamma},\boldsymbol{\delta})$$

$$= \frac{\sum_V (\nu^{\rm sp}_V/(-E_{0B}(\boldsymbol{\eta},\boldsymbol{\gamma},\boldsymbol{\delta})+V))\partial_{\delta_{i\sigma}}V}{\sum_V \nu^{\rm sp}_V/(-E_{0B}(\boldsymbol{\eta},\boldsymbol{\gamma},\boldsymbol{\delta})+V)}. \tag{40}$$

The expressions in the second lines of (38)–(40) have been obtained by using the derivatives of equation (23), which for a generic parameter ξ read

$$-\sum_V \nu^{\rm sp}_V \partial_\xi \log\left(\frac{-E_{0B}+V}{\epsilon}\right) + \sum_T \nu^{\rm sp}_T \partial_\xi \log(T) = 0, \tag{41}$$

where $\boldsymbol{\nu}^{\rm sp}$ is given by (21) and is determined once $E_{0B}(\boldsymbol{\eta},\boldsymbol{\gamma},\boldsymbol{\delta})$ has been solved. Similar expressions hold for fermions by using the derivatives of equation (35):

$$-\sum_V \nu^{\rm sp}_V \partial_\xi \log\left(\frac{-E_{0F}+V}{\epsilon}\right) + \sum_T \nu^{\rm sp}_T \partial_\xi \log(T) + \partial_\xi \log\left(\frac{E^{(0)}_{0F}}{E^{(0)}_{0B}}\right) = 0. \tag{42}$$

(ii) If the operator O is not a term of the Hamiltonian H, we consider a new Hamiltonian $H(\xi) = H + \xi O$ and calculate the corresponding ground-state energy $E_0(\xi)$. Note that, since the used probabilistic representation holds for any system described by a finite Hamiltonian matrix [4], the nature of the operator O is arbitrary. As an example, we study the spin–spin structure factor

$$S(q_x,q_y) = \frac{1}{|\Lambda|}\sum_{i,j\in\Lambda} {\rm e}^{{\rm i}q_x(x_i-x_j)+{\rm i}q_y(y_i-y_j)}\langle E_0|S_iS_j|E_0\rangle, \tag{43}$$

where $S_i = c^\dagger_{i\uparrow}c_{i\uparrow} - c^\dagger_{i\downarrow}c_{i\downarrow}$ and x_i and y_i are the coordinates of the ith lattice point. The quantum expectation of the operators S_iS_j in the ground state of the hard-core boson FNU model, $\langle E_{0B}(\epsilon,\gamma)|S_iS_j|E_{0B}(\epsilon,\gamma)\rangle$, can be obtained by considering the Hamiltonians

$$H(\xi_{ij}) = H + \xi_{ij}S_iS_j, \tag{44}$$

where H represents the FNU model. For these Hamiltonians, the possible values of the potential are $V = m\gamma + k\xi_{ij}$, with $m = 0, 1, \ldots, N_p$ and $k = -1, 0, 1$, and we have

$$\begin{aligned}\langle E_{0B}(\epsilon,\gamma)|S_iS_j|E_{0B}(\epsilon,\gamma)\rangle &= \partial_{\xi_{ij}}E_{0B}(\epsilon,\gamma,\xi_{ij})|_{\xi_{ij}=0}\\ &= \left.\frac{\sum_V(\nu_V^{\mathrm{sp}}/(-E_{0B}(\epsilon,\gamma,\xi_{ij})+V))\partial_{\xi_{ij}}V}{\sum_V \nu_V^{\mathrm{sp}}/(-E_{0B}(\epsilon,\gamma,\xi_{ij})+V)}\right|_{\xi_{ij}=0},\end{aligned} \tag{45}$$

where $E_{0B}(\epsilon,\gamma,\xi_{ij})$ is the ground-state energy of the Hamiltonian (44) and is calculated as explained in section 4.1.

6. Numerical results

We now apply the approach developed in the previous sections to some example cases. In particular, we compare the ground-state energy obtained by equations (28) and (35) with that from exact numerical calculations.

In our approach, the starting point is the evaluation of the statistical moments $\bar{\boldsymbol{\nu}}$ and $\boldsymbol{\Sigma}$. These are obtained by generating trajectories in the lattice configuration space and counting the multiplicities N_V and N_A. The length of the trajectories is chosen to be sufficiently large for the asymptotic behaviour to be established. The determination of $\bar{\boldsymbol{\nu}}$ and $\boldsymbol{\Sigma}$ with good statistical precision requires a number of trajectories, which increases no more than linearly with the number of lattice sites $|\Lambda|$. Therefore, the evaluation of these moments is feasible even for large systems. In the following applications, the statistical errors associated with the measurement of $\bar{\boldsymbol{\nu}}$ and $\boldsymbol{\Sigma}$ are negligible on the scales considered.

In figure 1, we show the behaviour of E_{0B} for the hard-core boson FNU model as a function of the interaction strength γ for several lattice systems. The solution of equation (28) compares rather well with the results of exact diagonalizations or QMC simulations. There is a small systematic error which grows with increasing γ and/or the system size and which is maximum at half density. This error is related to the Gaussian shape (19) assumed for the asymptotic probability density. In fact, the mentioned central limit theorem for Markov chains applies to the variables $\nu_V\sqrt{N}$ and $\nu_A\sqrt{N}$, whereas the function g_N given by equation (17) depends on $\nu_V N$ and $\nu_A N$. This implies that the tails of the probability density give a finite contribution to the integral (20). Furthermore, from the structure of g_N, it is evident that this error becomes large when the components of the vector $\boldsymbol{u}$ assume large values, i.e. for large values of γ and/or large system sizes.

In figure 2, we show the behaviour of E_{0F} evaluated according to equation (35) as a function of the interaction strength γ for the same cases considered in figure 1. Compared with the hard-core boson case, we observe a further systematic error due to the approximation $s_N(\gamma) \simeq s_N(0)$. Depending on the particle density of the system, this error adds to or subtracts from the systematic error due to the Gaussian tails of the probability density discussed for hard-core bosons.

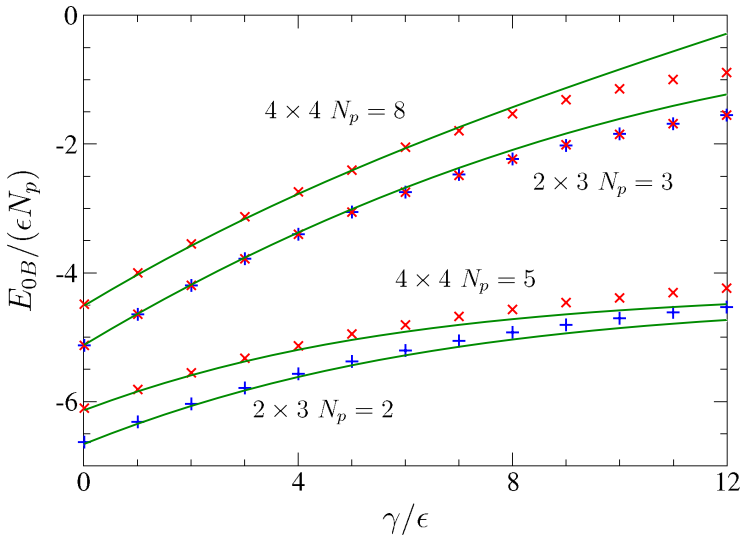

Figure 1. Ground-state energy per particle for the hard-core boson FNU model versus the interaction strength γ. The results from equation (28) (——) are compared with those from exact diagonalizations (+) and QMC simulations ($\times$) for two-dimensional systems with periodic boundary conditions and different $L_x \times L_y$ sites and $N_\uparrow = N_\downarrow = N_p$ particles. The statistical errors in the QMC data are negligible in this scale.

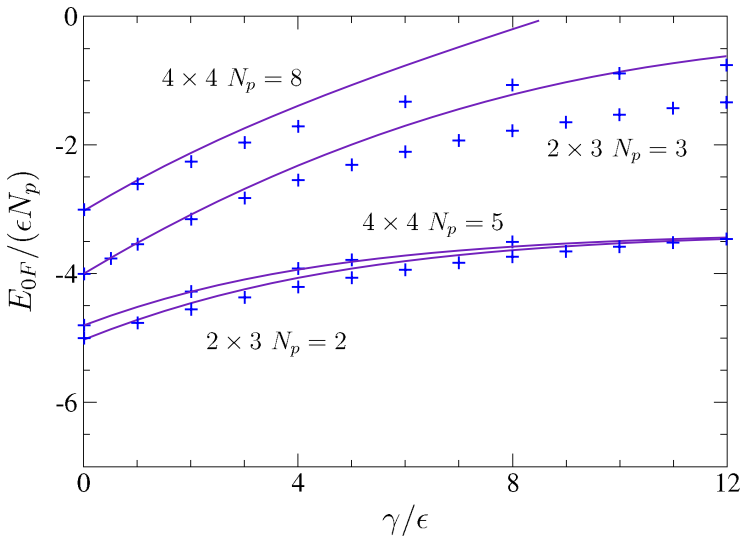

Figure 2. As in figure 1 for the fermion FNU model. In this case no QMC simulations are available. Exact diagonalization data for the 4×4 systems are taken from [15] ($N_p = 8$) and [16, 17] ($N_p = 5$).

We stress that, once $\bar{\boldsymbol{\nu}}$ and $\boldsymbol{\Sigma}$ are known, our approach provides any other ground-state quantity analytically as a function of the Hamiltonian parameters. On the other hand, QMC methods require, due to the unavoidable branching or reconfiguration techniques [7], different simulations for different values of the parameters.

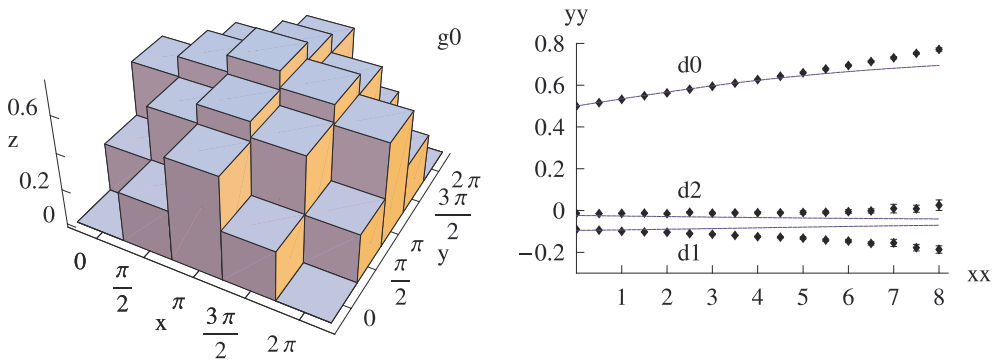

Figure 3. Spin–spin structure factor $S(q_x, q_y)$ for the hard-core boson FNU model at $\gamma = 0$ in a lattice with 4×4 sites, $N_\uparrow = N_\downarrow = 8$ particles and periodic boundary conditions. For the same system, on the right plot, we show the values of the ground-state expectation of the operators $S_i S_j$ for $d_{ij} = 0, 1, 2$ as a function of the interaction strength γ (solid lines) compared with Monte Carlo results (dots with error bars).

As an example of calculation of correlation functions in the ground state, in figure 3, we report the spin–spin structure factor $S(q_x, q_y)$ evaluated by using equations (43)–(45) for the hard-core boson FNU model. The value $S(\pi, \pi)$ represents a maximum for $S(q_x, q_y)$ and for large values of $|\Lambda|$ is related to the staggered magnetization m_s through $m_s = \sqrt{S(\pi, \pi)/|\Lambda|}$. Note that in the 4×4 system with periodic boundary conditions considered in figure 3, we have only five different values for $\langle E_0|S_i S_j|E_0\rangle$ corresponding to the five possible distances $d_{ij} = |x_i - x_j| + |y_i - y_j| = 0, 1, 2, 3, 4$. In figure 3, we also show the behaviour of $\langle E_0|S_i S_j|E_0\rangle$ as a function of γ for $d_{ij} = 0, 1, 2$. These terms provide the most important contributions to $S(\pi, \pi)$. For small values of γ, the results compare rather well with Monte Carlo data.

7. Conclusions

By using saddle-point techniques and a central limit theorem, we have exploited an exact probabilistic representation of the quantum dynamics in a lattice to derive analytical approximations for the matrix elements of the evolution operator in the limit of long times. For both hard-core boson and fermion systems, this development yields to a simple scalar equation for the ground-state energy. This equation depends on the values of the generalized potentials V and of the kinetic quantities T, and on the statistical moments $\bar{\boldsymbol{\nu}}$ and $\boldsymbol{\Sigma}$ of their asymptotic multiplicities N_V and N_T. In turn, these moments depend only on the structure of the system Hamiltonian, not on the values of the Hamiltonian parameters. This implies that the statistical moments must be measured *una tantum* for a given Hamiltonian structure and, once $\bar{\boldsymbol{\nu}}$ and $\boldsymbol{\Sigma}$ are known, our approach provides the ground-state energy analytically as a function of the Hamiltonian parameters.

In the long-time limit, the saddle-point integrations used in our approach are asymptotically exact and the central limit theorem evoked applies rigorously to the rescaled multiplicities $N_V/\sqrt{N}$ and $N_T/\sqrt{N}$. However, since functions depending on N_V and N_T are involved, we have a small systematic error related to the finite contributions from the tails of the probability

density. This systematic error could be reduced by a large deviation analysis. In fact, equations (27) and (28) suggest that the Gaussian approximation for the probability density corresponds to a second-order truncation of a cumulant expansion. Anyway, the present Gaussian approach has the following relevant features: (i) the equations derived for the ground-state energy and the ground-state correlation functions are particularly simple; and (ii) the corresponding results compare rather well with the exact ones in regions of physical interest.

In the present paper, we have considered two-dimensional lattice models at imaginary times. Our approach, however, is valid in any dimension. Similar analytical expressions can be obtained also for the real time evolution.

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