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# Four electrons in a two-leg Hubbard ladder: exact ground states

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**Abstract**
In the case of a two-leg Hubbard ladder we present a procedure which allows the exact deduction of the ground state for the four-particle problem in an arbitrary large lattice system, in a tractable manner, which involves only a reduced Hilbert space region containing the ground state. In the presented case, the method leads to nine analytic, linear and coupled equations providing the ground state. The procedure which is also applicable to few particle problems and other systems is based on an **r**-space representation of the wavefunctions and construction of symmetry adapted orthogonal basis wave vectors describing the Hilbert space region containing the ground state. Once the ground state is deduced, a complete quantum-mechanical characterization of the studied state can be given. Since the analytic structure of the ground state becomes visible during the use of the method, it is important not only to the understanding of theoretical aspects connected to exact descriptions or potential numerical approximation scheme developments, but is also relevant for a large number of potential technological application possibilities placed between nano-devices and quantum calculations, where the few particle behaviour and deep understanding are important key aspects.

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## 1. Introduction

In condensed matter context, experiments or related theoretical interpretations we often encounter a small number of particles confined in a system or device, for example, in the case of quantum dots [1], quantum well structures [2], mesoscopic systems [3], experimental entanglement [4], micro-crystals [5], cold gases trapped in optical lattices [6, 7], optical bound states [8], segregation [9], interfacial stress and fracture [10], self-organized structures [11], sintering [12], or compounds studied in the low concentration limit [13]. Such problems, presenting both theoretical [14–17] and technological [9, 10, 12, 18–20] interests have continuously attracted increasing attention. Starting from even one-electron problems solved exactly [17], several cases of interest for two [21–26], three [14, 15, 27–29], four [30–32] or few [33–35] particles have been studied, concentrating on the model behaviour in the low concentration limit, or motivated by experimentally measured characteristics. In this hierarchy of the increasing number of carriers in the study of a given problem, the particle number four ($N_p = 4$) represents a special case, since it is close to the particle number limit around which one can hope that deep rigorous descriptions can be made [36] even in the non-integrable cases, the problem is also treatable from the numerical side as well [37], statistics and $T \neq 0$ characterization can be given [38], and the problem retains even many-body aspects of the system's behaviour [39–41].

The simulations on the $N_p = 4$ particle problem started more than a decade ago [37, 42], but up to today, only few valuable results are known in this subject in the condensed matter context, as follows. The energy dependence of the maximal Lyapunov exponent has been studied for 1D Lenard–Jones system [43], the spinless fermion case has been analysed as a simplified model for correlated electrons [30, 31], the conjecture of the Andreev–Lifshitz supersolid has been studied [32], entangled states have been described in the high frequency region [44], doped quantum well structures have been investigated [2], special cases where only two pairs of particles interact on a lattice were considered [45], localization lengths have been estimated in 1D disordered systems [3], and the behaviour in the presence of Coulomb forces has been analysed [46]. As can be seen, the knowledge accumulated in this direction is relatively poor. Approximated procedures have been applied under different conditions for different systems of interest, but the level of exact characteristics has not been reached yet.

The need to study at exact level system holding $N_p = 4$ particles is enhanced by several motivations. First of all, $N_p = 4$ is placed in the low-density limit, and as known, in this limit, especially in low dimensions, no class of diagrams can be neglected in describing the system [47]. Given by this difficulty, one often finds that traditional approximation schemes which work at higher densities here fail [48] or provide unphysical results [49]. Secondly, we are placed in the concentration limit where the formation of Fermi liquid properties can be studied [30], and since this parameter region is usually numerically accessible, research with analytical focus, starting from numerical results, also can be done. Thirdly, as several times have been accentuated [50, 51], key aspects of the unapproximated descriptions are often hidden in the few-particle cases. The four-particle case seems to be tractable also from this point of view. Finally, in $N_p = 4$ case we face a situation which experimentally is produced, having potential application possibilities in several areas, as for example in the study of entangled states [52], non-local character of quantum theory [53], high precision spectroscopy [54], quantum communication, quantum cryptography, and quantum computation [55] fields where deep and high quality results are clearly demanded [57].

Starting from the motivations presented above, we show in this paper that for the $N_p = 4$ case, exact, analytical and explicit results holding essential information about the system behaviour can indeed be provided, even for arbitrary large systems. To show this, we present below the exact ground state for four interacting electrons placed in an arbitrary large two-leg Hubbard ladder described by periodic boundary conditions. This is given in conditions for which, even the known three (quantum-mechanical) particle exact results are very rare for systems taken outside one dimension (see [29] and the references therein); hence we hope that the presented results will generate creative advancements.

In order to obtain such results, a direct space representation is used for the wavefunctions. Starting from local particle configurations, symmetry adapted ortho-normalized basis wave vectors are constructed. Based on these, in the studied case, an explicit and analytic closed system of nine equations is constructed, whose secular equation provides the ground-state wavefunction and energy. Deducing the ground-state wavefunction for different microscopic parameters of the model, ground-state expectation values are calculated for different physical quantities of interest, and correlation functions are deduced in order to characterize the ground-state properties.

The method which is described here is in principle not model or particle number dependent, and could be applied for other systems as well. In presenting our calculations, the aim was not to hide the obtained results behind a numerical treatment or deduced symmetry properties, (which certainly also can be done), but to show clear, visible and explicit properties which, based on the provided essential characteristics, could enhance further creative thinking or applications. In order to underline the importance of these aspects we note, for example, that in recent studies made for states containing two to four particles, especially in attempts to characterize the entanglement [52], or quantum dots [56], often the analysis must be made without knowing the state completely [57][1]. We show below how such ingredients, at least at the level of the ground state, are possible to overcome.

The remaining part of the paper is structured as follows. Section 2 presents the Hamiltonian, the deduction procedure and the ground-state wavefunctions. Section 3 exemplifies the physical properties of the ground state. Section 4 presents the summary and conclusions of the paper, while appendices A and B presenting mathematical details close the presentation.

## 2. Hamiltonian and ground-state wavefunctions

The strategy which we use for presentation is the following one. We have chosen a simple model which allows us to characterize the construction of exact ground states in the presence of four particles. After presenting the results we indicate how the procedure could be applied for other systems as well.

### *2.1. Presentation of the Hamiltonian*

The Hamiltonian we use for the presentation has the form of a standard two-leg Hubbard ladder Hamiltonian

$$\hat{H} = -t_{\parallel} \sum_{<i,j>_{\parallel},\sigma} \left(\hat{c}^{\dagger}_{i,\sigma}\hat{c}_{j,\sigma} + \mathrm{H.c.}\right) - t_{\perp} \sum_{<i,j>_{\perp},\sigma} \left(\hat{c}^{\dagger}_{i,\sigma}\hat{c}_{j,\sigma} + \mathrm{H.c.}\right) + U \sum_{i} \hat{n}_{i,\uparrow}\hat{n}_{i,\downarrow}, \tag{1}$$

where $\hat{c}^{\dagger}_{i,\sigma}$ creates an electron at site $i$ with spin $\sigma$, $t_\alpha$ holding the index $\alpha = \parallel, \perp$ are nearest-neighbour hopping amplitudes along and perpendicular to ladder legs, $U$ is the on-site Coulomb interaction and $\langle i, j\rangle_\alpha$ represents nearest-neighbour sites in $\alpha$ direction taken into account in the sum over the lattice sites only once.

### *2.2. The construction of the basis wave vectors*

If we would like to analyse by exact diagonalization the four-particle problem in the singlet case in a two-leg Hubbard ladder containing $N$ lattice sites, we must treat numerically a Hilbert space of $d_H = [N(N-1)/2]^2$ dimensions, where for example at $N = 30$ we have $d_H = 2.16 \times 10^5$, and for $N \to \infty$ one encounters $d_H \to \infty$ as $d_H \sim N^4$.

We show below how it is possible to deduce exactly the ground state for a such type of system in the case of an arbitrary large two-leg Hubbard ladder based on only nine linear and analytic equations, and to extract essential information from the obtained results. In order to

[1] We note that the here deduced ground states are entangled in the sense that cannot be factorized into a product of single-particle wavefunctions, although the constituent particles are entirely distinct, see [52].

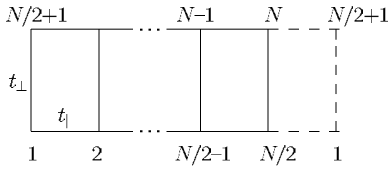


**Figure 1.** The numbering of the lattice sites for the two-leg ladder taken with periodic boundary conditions. $N$ denoting the number of lattice sites is considered even. The $t_\perp (t_\|)$ denotes the inter-leg (intra-leg) hopping matrix element.

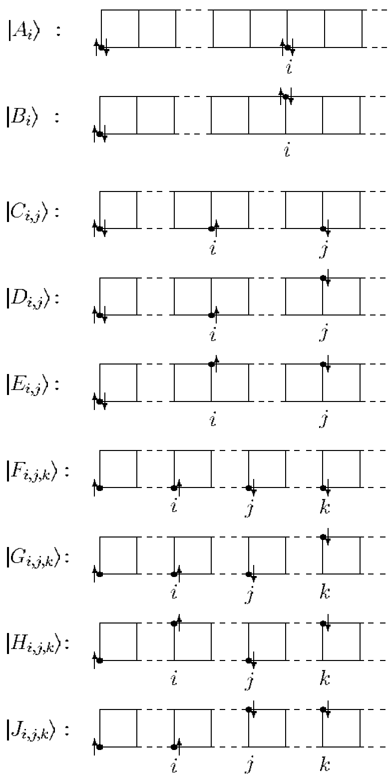


**Figure 2.** The different possible types of base vectors. We note that for the cases $C$, $E$ $i \neq j$, while for $F$, $J$ $j < k$ is considered. In the cases $F$, $G$, $H$, $J$, the double occupancy is forbidden.

do this, first we delimit exactly the Hilbert space region ($\mathcal{H}_g$) containing the ground state by the construction of nine types of orthogonal basis wave vectors spanning $\mathcal{H}_g$. This procedure is presented below.

*2.2.1. The generating configurations.* We are interested first to have an image about the possible type of states of the studied four particles in the system under consideration. To obtain such type of information, we number all lattice sites of the ladder as shown in figure 1 (periodic boundary conditions are considered). In the figure, $N$, considered even number, denotes the number of sites within the system, while $n = N/2$ gives the number of rungs. Using now an **r**-space representation, one observes that since the ladder legs, and the spin reversed configurations are equivalent, the studied four particles can be placed into the system only in nine possible ways, as depicted in figure 2. The presented possibilities, denoted by

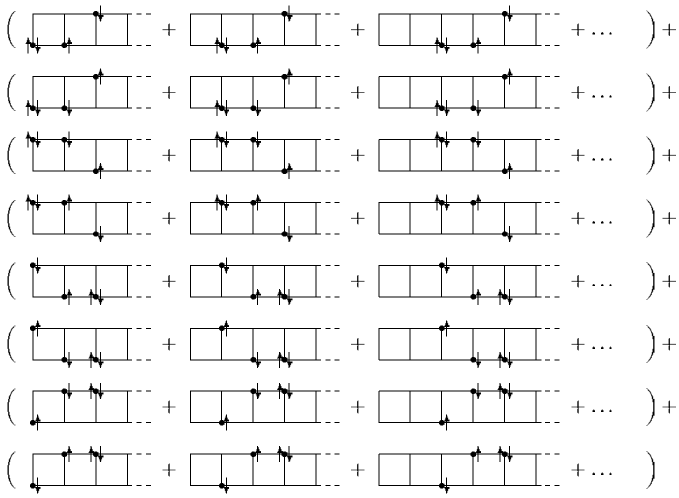

**Figure 3.** The structure of the $|D_{2,3}\rangle$ base vector.

capital letters $A$ to $J$, will provide nine types of basis wave vectors (denoted by the same letters), whose construction is presented below. We mention that the subscripts $i$, $j$, $k$ denote particle positions within the considered states $A$ to $J$ presented in figure 2, which are such chosen, to have the first particle position placed into the origin (e.g. lattice site 1). In the following, the nine possible four-particle states presented in figure 2 will be called *generating configurations*. How one arrives from the generating configuration $X = A, B, \ldots, J$ to the base vector $|X\rangle$, is explained in the following two subsections.

*2.2.2. The sum of configurations related to each generating configuration.* Each generating configuration provides other seven related configurations (brother configurations) of the same type. These are obtained by (a) rotating the generating configuration by 180° along the longitudinal symmetry axis of the ladder, (b) rotating the generating configuration by 180° along the symmetry axis perpendicular to the ladder, (c) rotating by 180° the configuration obtained at (b) along the longitudinal symmetry axis of the ladder, and finally, (d) other four related configurations are obtained by reversing all spin orientations in the generating configuration and the configurations deduced at points (a)–(c). As an example, the eight related configurations describing the state $D_{i,j}$ taken at $i = 2$, $j = 3$, are depicted in the first column of figure 3.

After this step, since all lattice sites are equivalent, the different 'related' configurations are translated by *elementary translation* $N/2$ times along the ladder, and all the contributions are added. We obtain in this manner a sum of configurations for each generating configuration. Such a sum contains $8 \times N/2$ components. For example, in the case of the $D_{2,3}$ state, this sum is presented in figure 3.

The procedure described above must be effectuated separately for each generating configuration. As a result, we obtain at this point nine configuration sums. Each of these sums will give rise to one basis wave vector as follows.

*2.2.3. The basis wave vectors.* A given configuration sum described in the previous subsection provides one basis wave vector if each individual configuration of the sum is written in mathematical form via four creation operators acting on the bare vacuum. In order to do this, we have to fix the order of creation operators for each type of contribution, which has been done as follows. For two doubly occupied sites we write the creation operators of the couples next to each other, first the spin up, then the spin down contribution, as $\hat{c}^\dagger_{i,\uparrow}\hat{c}^\dagger_{i,\downarrow}\hat{c}^\dagger_{j,\uparrow}\hat{c}^\dagger_{j,\downarrow}|0\rangle$, where only the restriction $i \neq j$ exists. In the case of basis wave vectors containing only one doubly occupied site at $i$ one uses $\hat{c}^\dagger_{i,\uparrow}\hat{c}^\dagger_{i,\downarrow}\hat{c}^\dagger_{j,\uparrow}\hat{c}^\dagger_{k,\downarrow}|0\rangle$, where $i \neq j$ and $i \neq k$ must hold. Finally, for cases without double occupancies, the convention $\hat{c}^\dagger_{i,\uparrow}\hat{c}^\dagger_{j,\uparrow}\hat{c}^\dagger_{k,\downarrow}\hat{c}^\dagger_{l,\downarrow}|0\rangle$ is considered, where $i < j$ and $k < l$ must hold. Using these conventions, for example, in the case of $|D_{i,j}\rangle$, taken at $i = 2$, $j = 3$ and depicted in figure 3 the result becomes

$$
\begin{aligned}
|D_{2,3}\rangle = {} & \big(\big(\hat{c}^\dagger_{1\uparrow}\hat{c}^\dagger_{1\downarrow}\hat{c}^\dagger_{2\uparrow}\hat{c}^\dagger_{(n+3)\downarrow} + \hat{c}^\dagger_{2\uparrow}\hat{c}^\dagger_{2\downarrow}\hat{c}^\dagger_{3\uparrow}\hat{c}^\dagger_{(n+4)\downarrow} + \hat{c}^\dagger_{3\uparrow}\hat{c}^\dagger_{3\downarrow}\hat{c}^\dagger_{4\uparrow}\hat{c}^\dagger_{(n+5)\downarrow} + \cdots\big) \\
& + \big(\hat{c}^\dagger_{1\uparrow}\hat{c}^\dagger_{1\downarrow}\hat{c}^\dagger_{(n+3)\uparrow}\hat{c}^\dagger_{2\downarrow} + \hat{c}^\dagger_{2\uparrow}\hat{c}^\dagger_{2\downarrow}\hat{c}^\dagger_{(n+4)\uparrow}\hat{c}^\dagger_{3\downarrow} + \hat{c}^\dagger_{3\uparrow}\hat{c}^\dagger_{3\downarrow}\hat{c}^\dagger_{(n+5)\uparrow}\hat{c}^\dagger_{4\downarrow} + \cdots\big) \\
& + \big(\hat{c}^\dagger_{(n+1)\uparrow}\hat{c}^\dagger_{(n+1)\downarrow}\hat{c}^\dagger_{(n+2)\uparrow}\hat{c}^\dagger_{3\downarrow} + \hat{c}^\dagger_{(n+2)\uparrow}\hat{c}^\dagger_{(n+2)\downarrow}\hat{c}^\dagger_{(n+3)\uparrow}\hat{c}^\dagger_{4\downarrow} + \hat{c}^\dagger_{(n+3)\uparrow}\hat{c}^\dagger_{(n+3)\downarrow}\hat{c}^\dagger_{(n+4)\uparrow}\hat{c}^\dagger_{5\downarrow} + \cdots\big) \\
& + \big(\hat{c}^\dagger_{(n+1)\uparrow}\hat{c}^\dagger_{(n+1)\downarrow}\hat{c}^\dagger_{3\uparrow}\hat{c}^\dagger_{(n+2)\downarrow} + \hat{c}^\dagger_{(n+2)\uparrow}\hat{c}^\dagger_{(n+2)\downarrow}\hat{c}^\dagger_{4\uparrow}\hat{c}^\dagger_{(n+3)\downarrow} + \hat{c}^\dagger_{(n+3)\uparrow}\hat{c}^\dagger_{(n+3)\downarrow}\hat{c}^\dagger_{5\uparrow}\hat{c}^\dagger_{(n+4)\downarrow} + \cdots\big) \\
& + \big(\hat{c}^\dagger_{3\uparrow}\hat{c}^\dagger_{3\downarrow}\hat{c}^\dagger_{2\uparrow}\hat{c}^\dagger_{(n+1)\downarrow} + \hat{c}^\dagger_{4\uparrow}\hat{c}^\dagger_{4\downarrow}\hat{c}^\dagger_{3\uparrow}\hat{c}^\dagger_{(n+2)\downarrow} + \hat{c}^\dagger_{5\uparrow}\hat{c}^\dagger_{5\downarrow}\hat{c}^\dagger_{4\uparrow}\hat{c}^\dagger_{(n+3)\downarrow} + \cdots\big) \\
& + \big(\hat{c}^\dagger_{3\uparrow}\hat{c}^\dagger_{3\downarrow}\hat{c}^\dagger_{(n+1)\uparrow}\hat{c}^\dagger_{2\downarrow} + \hat{c}^\dagger_{4\uparrow}\hat{c}^\dagger_{4\downarrow}\hat{c}^\dagger_{(n+2)\uparrow}\hat{c}^\dagger_{3\downarrow} + \hat{c}^\dagger_{5\uparrow}\hat{c}^\dagger_{5\downarrow}\hat{c}^\dagger_{(n+3)\uparrow}\hat{c}^\dagger_{4\downarrow} + \cdots\big) \\
& + \big(\hat{c}^\dagger_{(n+3)\uparrow}\hat{c}^\dagger_{(n+3)\downarrow}\hat{c}^\dagger_{(n+2)\uparrow}\hat{c}^\dagger_{1\downarrow} + \hat{c}^\dagger_{(n+4)\uparrow}\hat{c}^\dagger_{(n+4)\downarrow}\hat{c}^\dagger_{(n+3)\uparrow}\hat{c}^\dagger_{2\downarrow} + \hat{c}^\dagger_{(n+5)\uparrow}\hat{c}^\dagger_{(n+5)\downarrow}\hat{c}^\dagger_{(n+4)\uparrow}\hat{c}^\dagger_{3\downarrow} + \cdots\big) \\
& + \big(\hat{c}^\dagger_{(n+3)\uparrow}\hat{c}^\dagger_{(n+3)\downarrow}\hat{c}^\dagger_{1\uparrow}\hat{c}^\dagger_{(n+2)\downarrow} + \hat{c}^\dagger_{(n+4)\uparrow}\hat{c}^\dagger_{(n+4)\downarrow}\hat{c}^\dagger_{2\uparrow}\hat{c}^\dagger_{(n+3)\downarrow} \\
& + \hat{c}^\dagger_{(n+5)\uparrow}\hat{c}^\dagger_{(n+5)\downarrow}\hat{c}^\dagger_{3\uparrow}\hat{c}^\dagger_{(n+4)\downarrow} + \cdots\big)\big)|0\rangle
\end{aligned}
$$

Similar procedure applies for all basis wave vectors. We mention that the so obtained basis wavefunctions are orthogonal.

Here we must note that because of the fixed conventions presented above, sometimes an additional negative sign arises in the process of writing the mathematical expression corresponding to a basis wave vector component translated from the end to the beginning of the ladder in the presence of the periodic boundary conditions. For example, if we translate the vector $\hat{c}^\dagger_{1,\uparrow}\hat{c}^\dagger_{N/2,\uparrow}\hat{c}^\dagger_{2,\downarrow}\hat{c}^\dagger_{3,\downarrow}|0\rangle$ by an elementary translation along the ladder, according to the fixed conventions one obtains $\hat{c}^\dagger_{2,\uparrow}\hat{c}^\dagger_{1,\uparrow}\hat{c}^\dagger_{3,\downarrow}\hat{c}^\dagger_{4,\downarrow}|0\rangle = -\hat{c}^\dagger_{1,\uparrow}\hat{c}^\dagger_{2,\uparrow}\hat{c}^\dagger_{3,\downarrow}\hat{c}^\dagger_{4,\downarrow}|0\rangle$.

### 2.3. *The ground-state wavefunction*

After the calculation presented above, we are in the possession of nine types of orthogonal basis wave vectors $|A_i\rangle, |B_i\rangle, \ldots, |J_{i,j,k}\rangle$, enumerated together with their generating configuration in figure 2. Let us denote these basis wave vectors by $\big|O^{(m)}_{i,j,..}\big\rangle$, $m = 1, 2, 3, \ldots, 9$. Now one observes that by applying the Hamiltonian on a given $\big|O^{(m)}_{i,j,..}\big\rangle$ basis wave vector with fixed $m$, we obtain the result inside the $\big\{\big|O^{(m)}_{i,j,..}\big\rangle\big\}$ set. Consequently, nine explicitly given analytic linear equations form a closed system of equations, whose secular equation, by its minimum eigenvalue, contains the ground state at attractive $U$. The nine equations are exemplified in appendix A and are available in their complete extent in [58]. The ground-state nature of the minimum energy eigenstate has been tested by exact numerical diagonalizations taken on the full Hilbert space for different $N$ values.

The fact that the analytic solution of the problem can be given in such a manner for arbitrary large ladder length is connected to the observation that with increasing $N$, the type of the particle configurations describing the system (see figure 2) remains unchanged. The deduction of the ground state itself from the system of equations presented in appendix A must be numerically given[2]. Since the possible inter-particle distances (e.g. the possible values of the $i, j, \ldots$ indices in $O^{(m)}_{i,j,\ldots}$ at fixed $m$) depend on the $N$ value, the number of equations which must be numerically treated depends on $N$ in the frame of the same analytic expressions. For example, for the $m = 1$ case we have $1 < i \leqslant 1 + N/4$, for the $m = 2$ case we have $1 \leqslant i \leqslant 1 + N/4$, etc. The number of obtained equations $d_e$ is however significantly lower than $d_H$, the $c_g = d_H/d_e$ ratio being at least of order $10^2$ at intermediate $N \sim O(10)$ values. Increasing $N$, $c_g$ further increases.

### *2.4. Application possibilities in other cases*

In fact, the deduced system of equations, based on symmetry properties, delimitates from the full Hilbert space a $d_e$ dimensional space region, inside of which the ground state is placed. The deduction of such a region is possible for other (non-disordered) models, and for other particle numbers as well. In order to do this, we mention that if the lattice sites are equivalent, the elementary translation of a particle configuration can, in principle, be given with a site-independent multiplicative phase factor $\exp(\mathrm{i}\alpha_{\mathrm{trans}})$. Furthermore, the rotation of a particle configuration along a symmetry axis can be given, in principle, with a multiplicative phase factor of the form $\exp(\mathrm{i}\alpha_{\mathrm{rot}})$, both $\alpha_{\mathrm{trans}}, \alpha_{\mathrm{rot}}$ providing their contributions in the basis wave vectors[3]. In the described case, we have $\alpha_{\mathrm{trans}} = \alpha_{\mathrm{rot}} = 0$, but in other cases, the energy can be minimized in function of these parameters.

In deducing the linear system of equations describing $\mathcal{H}_g$ in a new case characterized by a new $\hat{H}$, one must start from a given basis wave vector (denoted by $|v_1\rangle$, for example). This is obtained from a generating particle configuration, which is translated and rotated as specified above, all such obtained configurations being summed up. From technical reasons, the first generating particle configuration must be such chosen to contain (for 1/2 spin fermions) only double occupied sites placed in nearest-neighbour sites. Calculating now $\hat{H}|v_1\rangle$, the result becomes a linear combination containing new base vectors $|v_2\rangle, \ldots, |v_{n_1}\rangle$, holding the same symmetry properties, but being related to new generating configurations. Continuing the procedure by calculating $\hat{H}|v_2\rangle$, $|\hat{H}|v_3\rangle$, etc, since periodic boundary conditions are used, the linear system of equations closes up. It is even not important to know all distinct particle configuration possibilities, since these are automatically generated by the $\hat{H}|v_i\rangle$ operation.

## 3. Ground-state properties

By diagonalizing the system of equations presented in appendix A and taking the minimum energy solution, one finds the ground-state wavefunction $|\Psi_g\rangle$. Using this, the complete quantum-mechanical characterization of the ground state can be given. In order to exemplify the results, we present in (B.1), (B.2) explicit expressions containing the leading terms of the ground-state wavefunction for two parameter values. Even appendix B shows that in the leading terms of the ground-state wavefunction, the particles have the tendency to be placed in pairs, the pairs tending to occupy the highest possible distance between them. This is reflected as well in the density–density correlation function depicted in figure 4(*c*).

Ground-state expectation values and correlation functions are exemplified in figures 4 and 5, calculated for $N = 28$, e.g. ladder containing 14 rungs described by periodic boundary conditions taken along the ladder. The correlation functions are defined as follows.

[2] Such property is present also in the case of the Bethe Ansatz.
[3] The $\alpha_{\mathrm{trans}}$ and $\alpha_{\mathrm{rot}}$ angles can be connected to the momentum and angular momentum values in the ground state.

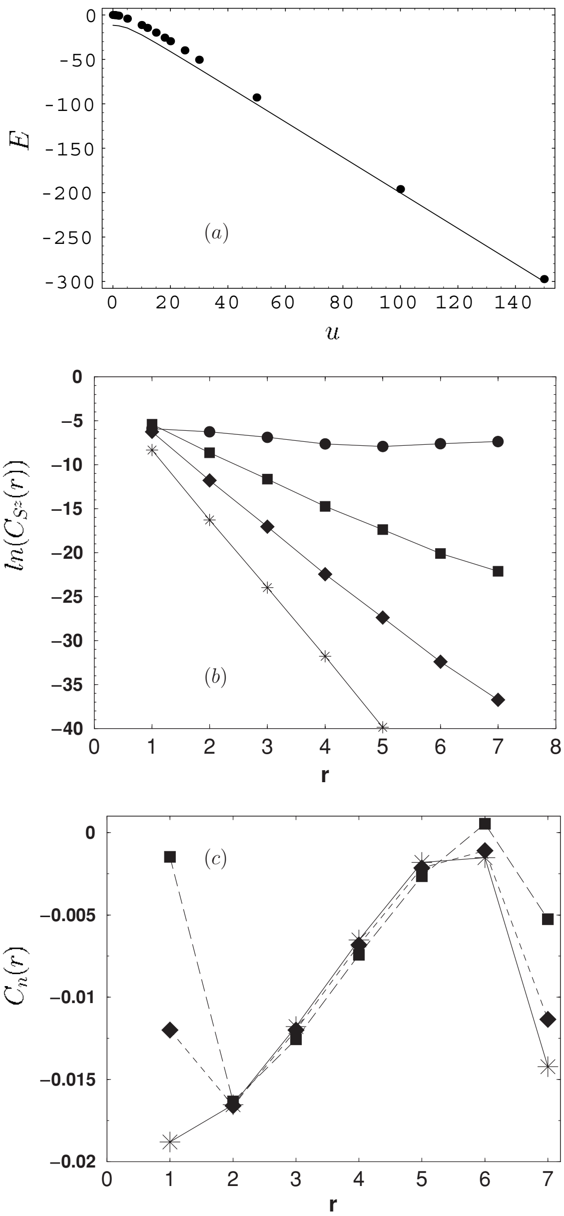


**Figure 4.** The properties of the ground state for $t_\perp = t_\parallel$. (*a*) The dependence of the energy (in $t_\parallel$ units) on $u = U/t_\parallel$. The continuous line is the total energy, while the dots indicate the potential energy. (*b*) The logarithm of the same-leg $\hat{S}^z$–$\hat{S}^z$ correlation function for $u = 0$ (dots, dot-dashed line), $u = -10$ (squares, long dashed line), $u = -30$ (diamonds, short dashed line), $u = -100$ (stars, continuous line). (*c*) The same-leg density–density correlation function for $u = 0$ (dots, dot-dashed line), $u = -10$ (squares, long dashed line), $u = -30$ (diamonds, short dashed line), $u = -100$ (stars, continuous line).

The density–density correlation function has the expression

$$C_n(r) = \frac{1}{N}\sum_{i=1}^{N}(\langle \hat{n}_i \hat{n}_{i+r}\rangle - \langle \hat{n}_i\rangle\langle \hat{n}_{i+r}\rangle) \tag{2}$$

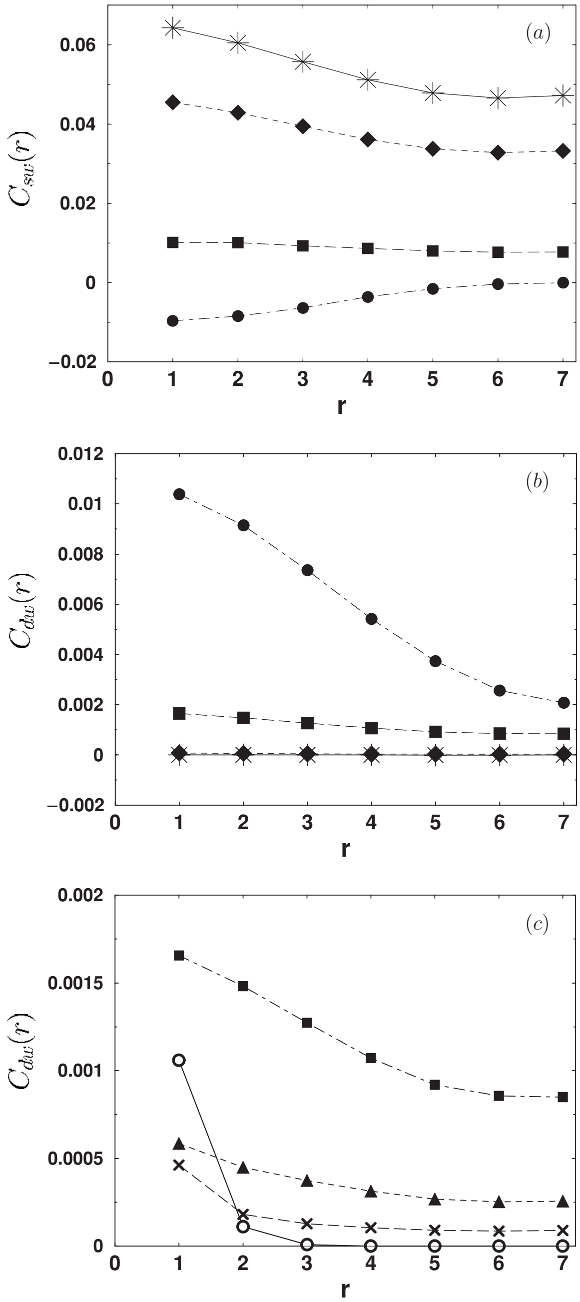


**Figure 5.** Superconducting ground-state correlation functions. (*a*) The same-leg superconducting s-wave correlation function for $t_\perp = t_\parallel$ and $u = 0$ (dots, dot-dashed line), $u = -10$ (squares, long dashed line), $u = -30$ (diamonds, short dashed line), $u = -100$ (stars, continuous line). (*b*) The superconducting d-wave correlation function for $t_\perp = t_\parallel$ and $u = 0$ (dots, dot-dashed line), $u = -10$ (squares, long dashed line), $u = -30$ (diamonds, short dashed line), $u = -100$ (stars, continuous line). We mention that the curves corresponding to the last two $u$ values are almost superposed. (*c*) Superconducting d-wave correlation function for $u = -10$ and $t = t_\perp/t_\parallel$ taken as $t = 1$ (squares, dot-dashed line), $t = 0.5$ (triangles, short dashed line), $t = 0.3$ (X-s, long dashed line), $t = 0.01$ (circles, continuous line).

where $\hat{n}_i = \hat{n}_{i\uparrow} + \hat{n}_{i\downarrow}$, $\hat{n}_{i,\sigma} = \hat{c}^\dagger_{i\sigma}\hat{c}_{i\sigma}$. The spin correlations are studied via

$$C_{S^z}(r) = \frac{1}{N}\sum_{i=1}^{N}\left(\left\langle \hat{S}^z_i \hat{S}^z_{i+r}\right\rangle - \left\langle \hat{S}^z_i\right\rangle\left\langle \hat{S}^z_{i+r}\right\rangle\right), \tag{3}$$

where $\hat{S}^z = (1/2)(\hat{n}_{i,\uparrow} - \hat{n}_{i,\downarrow})$. The superconducting pairing s-wave [59] correlation function is

$$C_{sw}(r) = \frac{1}{N}\sum_{i=1}^{N}\left(\left\langle \hat{c}^\dagger_{i\uparrow}\hat{c}^\dagger_{i\downarrow}\hat{c}_{(i+r)\downarrow}\hat{c}_{(i+r)\uparrow}\right\rangle - \left\langle \hat{c}^\dagger_{i\uparrow}\hat{c}_{(i+r)\uparrow}\right\rangle\left\langle \hat{c}^\dagger_{i\downarrow}\hat{c}_{(i+r)\downarrow}\right\rangle\right), \tag{4}$$

and the superconducting pairing d-wave [60] correlations are studied via

$$C_{dw}(r) = \frac{1}{N}\sum_{i=1}^{N}\langle \hat{\Delta}^\dagger(i+r)\hat{\Delta}(i)\rangle \tag{5}$$

where $\hat{\Delta}(i) = (\hat{c}_{i_2\downarrow}\hat{c}_{i_1\uparrow} - \hat{c}_{i_2\uparrow}\hat{c}_{i_1\downarrow})$. The $i$ in $\hat{\Delta}(i)$ denotes a rung connecting the lattice sites $i_1, i_2$. The $r$ values inside the figures are given in lattice constant units.

Figure 4($a$) presents the ground-state energy and the potential energy in $t_\parallel$ units in function of $u = |U/t_\parallel|$ at $t_\parallel = t_\perp$. Figure 4($b$) shows that the spin–spin correlations are exponentially decreasing, the decrease rate in the $\exp(-r/\xi)$ being of the form $1/\xi = 0.34 + 0.78\sqrt{|u|}$. The density–density correlations depicted in figure 4($c$) show that the particles tend to occupy opposite positions in the ladder closed by periodic boundary conditions.

In figure 5 the behaviour of the superconducting correlation functions is presented. In these plots $u = U/t_\parallel$ holds. The correlations in figure 5 are decreasing with $r$, and for s-wave case slightly increase by increasing the attractive $U$ value. Figure 5($c$) further shows that the decrease of the inter-leg hopping amplitude at fixed on-site interaction is detrimental to d-wave pairing correlations. Similar behaviour has been found also by others [59].

## 4. Summary and conclusions

We describe a procedure which allows the exact deduction of ground-state wavefunctions for few particles in lattice models. The main result of our paper is that indeed, such a type of analytic description can be made. In the case of an arbitrary large two-leg Hubbard ladder taken with periodic boundary conditions and containing four electrons, presented in detail, the method leads for the singlet state to nine analytic linear and coupled closed system of equations, whose secular equation, through its minimum eigenvalue solution, provides the ground-state wavefunction and ground-state energy. The procedure is based on an **r**-space representation of the wavefunctions and properly constructed symmetry adapted orthogonal basis wave vectors. These are obtained from generating particle configurations translated and rotated in the lattice and finally added. The linear system of equations is obtained by applying the Hamiltonian on the deduced basis wave vectors. The procedure can be applied for other systems as well.

The fact that the analytic structure of the ground state becomes visible by the use of the method underlines that the presented procedure contributes not only to the understanding of theoretical aspects related to exact descriptions, or development possibilities of new numerical approximation schemes, but also has implications on a broad spectrum of subfields related to technological developments placed in between nano-devices and quantum computation, where the exact knowledge of the behaviour of a small number of quantum-mechanical particles plays a main role.

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## Appendix A. The linear system of equations containing the ground state

This appendix presents the nine analytic equations describing the action of the Hamiltonian on the basis wave vectors.

The first two equations are devoted to the $|A_i\rangle$, $|B_i\rangle$ species containing only (two) doubly occupied sites.

$$\begin{aligned}
\hat{H}|A_i\rangle &= 2u|A_i\rangle - t_\perp|D_{i,i}\rangle - I_{i>2}|C_{i-1,i}\rangle - I_{i\leqslant\frac{n}{2}}|C_{i,i+1}\rangle,\\
\hat{H}|B_i\rangle &= 2u|B_i\rangle - t_\perp I_{i>1}|D_{i,i}\rangle - I_{i>1}|E_{i-1,i}\rangle - I_{i\leqslant\frac{n}{2}}|E_{i,i+1}\rangle,
\end{aligned}$$

where $I_K = 1$ if the statement $K$ is true, and $I_K = 0$ otherwise.

The following three equations describe the action of $\hat{H}$ on the basis wave vectors containing only one doubly occupied site ($|C_{i,j}\rangle$, $|D_{i,j}\rangle$, $|E_{i,j}\rangle$) as follows

$$\begin{aligned}
\hat{H}|C_{i,j}\rangle = u|C_{i,j}\rangle &- 4\delta_{j,i+1}|A_i\rangle - 4\delta_{j,i+1}\big(1+\delta_{i,\frac{n}{2}}\big)|A_{i+1}\rangle - (1-\delta_{i,2})|C_{i-1,j}\rangle\\
&- \big(1-\delta_{j,i+1}-\delta_{i,2}\delta_{j,\frac{n+i}{2}+1}\big)|C_{i,j-1}\rangle - \big(1-\delta_{i,2}\delta_{j,\frac{n+i}{2}}+\delta_{j,n-i+1}-\delta_{j,n-i+2}\big)|C_{i,j+1}\rangle\\
&- (1-\delta_{j,i+1})(1+\delta_{j,n-i+1}-\delta_{j,n-i+2})|C_{i+1,j}\rangle\\
&+ \delta_{i,2}(1+\delta_{j,3})\big(1-\delta_{j,\frac{n+i}{2}}-\delta_{j,\frac{n+i}{2}+1}\big)|C_{2,n-j+3}\rangle\\
&- t_\perp|D_{i,j}\rangle - t_\perp\cdot\left\{\begin{matrix} I_{j\leqslant\frac{n}{2}+1}|D_{j,i}\rangle \\ I_{j>\frac{n}{2}+1}(1-\delta_{j,n-i+2})|D_{n-j+2,n-i+2}\rangle \end{matrix}\right\}\\
&- (1-\delta_{i,2})(1+\delta_{j,i+1})|F_{i-1,i,n-j+i+1}\rangle\\
&+ \left\{\begin{matrix} (1-\delta_{i,2})(1+\delta_{j,i+1})(1-\delta_{i,3}I_{j\geqslant\frac{n+i+1}{2}})|F_{i,2,j}\rangle \\ -\delta_{i,3}I_{j>\frac{n+i+1}{2}}|F_{i,2,n-j+i+1}\rangle \end{matrix}\right\}\\
&- (1+\delta_{j,i+1})(1+\delta_{j,n-i+1}-\delta_{j,n-i+2})|F_{i,i+1,n-j+i+1}\rangle\\
&+ (1+\delta_{j,i+1})(1+\delta_{j,n-i+1}-\delta_{j,n-i+2})\\
&\times \left\{\begin{matrix} (1-\delta_{i,2}I_{j\geqslant\frac{n+i}{2}})|F_{i+1,2,j+1}\rangle \\ -\delta_{i,2}I_{j>\frac{n+i}{2}}|F_{i+1,2,n-j+i+1}\rangle \end{matrix}\right\} + t_\perp\cdot\left\{\begin{matrix} -I_{j\leqslant\frac{n+i+1}{2}}|G_{i,j,1}\rangle \\ I_{j>\frac{n+i+1}{2}}|G_{i,n-j+i+1,i}\rangle \end{matrix}\right\}\\
&+ t_\perp(1-\delta_{j,n-i+2})\cdot\left\{\begin{matrix} I_{j\leqslant\frac{n}{2}+1}\cdot\left\{\begin{matrix} I_{j<2i-1}|G_{j,j-i+1,j}\rangle \\ -I_{j\geqslant 2i-1}|G_{j,i,1}\rangle \end{matrix}\right\} \\ I_{j>\frac{n}{2}+1}\cdot\left\{\begin{matrix} -I_{j\leqslant 2i-1}|G_{n-j+2,n-i+2,1}\rangle \\ I_{j>2i-1}|G_{n-j+2,n-j+i+1,n-j+2}\rangle \end{matrix}\right\} \end{matrix}\right\}.
\end{aligned}$$

$$\begin{aligned}
\hat{H}|D_{i,j}\rangle = u|D_{i,j}\rangle &- 4t_\perp\delta_{j,i}(|A_i\rangle + |B_i\rangle)\\
&- t_\perp(1-\delta_{j,1}-\delta_{j,i}+\delta_{j,n-i+2})\cdot\left\{\begin{matrix} I_{j\leqslant n-i+2}I_{j<i}(|C_{j,i}\rangle + |E_{j,i}\rangle) \\ I_{n-i+2\geqslant j>i}(|C_{i,j}\rangle + |E_{i,j}\rangle) \\ I_{j>n-i+2}(|C_{n-j+2,n-i+2}\rangle + |E_{n-j+2,n-i+2}\rangle) \end{matrix}\right\}\\
&+ \left\{\begin{matrix} -(1-\delta_{i,2})|D_{i-1,j}\rangle \\ \delta_{i,2}\big(1-\delta_{j,1}-\delta_{j,2}-\delta_{j,\frac{n+i}{2}}-\delta_{j,\frac{n+i}{2}+1}\big)|D_{i,n+i-j+1}\rangle \end{matrix}\right\}
\end{aligned}$$

$$
\begin{aligned}
&- \begin{Bmatrix} I_{j>1}\left[1-\delta_{i,2}\left(\delta_{j,2}+\delta_{j,\frac{n+i}{2}+1}\right)+\delta_{i,\frac{n}{2}+1}\delta_{j,2}\right]|D_{i,j-1}\rangle \\ \delta_{j,1}\left(1-\delta_{i,\frac{n}{2}+1}\right)|D_{i,n}\rangle \end{Bmatrix} \\
&- \begin{Bmatrix} \left[1-\delta_{i,2}\left(\delta_{j,1}+\delta_{j,\frac{n+i}{2}}\right)-\delta_{j,n}+\delta_{i,\frac{n}{2}+1}\left(\delta_{j,\frac{n}{2}}-\delta_{j,\frac{n}{2}+1}\right)\right]|D_{i,j+1}\rangle \\ \delta_{j,n}|D_{i,1}\rangle \end{Bmatrix} \\
&- \begin{Bmatrix} \left[I_{i<\frac{n}{2}}+\delta_{i,\frac{n}{2}}\left(I_{j<\frac{n}{2}+1}+\delta_{j,1}+2\delta_{j,\frac{n}{2}+1}\right)\right]|D_{i+1,j}\rangle \\ \left(\delta_{i,\frac{n}{2}}I_{j>\frac{n}{2}+1}+\delta_{i,\frac{n}{2}+1}(1-\delta_{j,1}-\delta_{j,i})\right)|D_{n-i+1,n-j+2}\rangle \end{Bmatrix} \\
&- (1-\delta_{i,2}) \begin{Bmatrix} I_{j\leqslant i}|G_{i-1,i,i-j+1}\rangle \\ I_{j>i}|G_{i-1,i,n-j+i+1}\rangle \end{Bmatrix} \\
&+ \begin{Bmatrix} \left[1-\delta_{i,2}-\delta_{i,3}\left(\delta_{j,2}+\delta_{j,3}+I_{j>\frac{n}{2}+1}\right)\right]|G_{i,2,j}\rangle \\ -\delta_{i,3}\delta_{j,3}|G_{i,2,1}\rangle \\ -\delta_{i,3}I_{j>\frac{n}{2}+2}|G_{i,2,n-j+i+1}\rangle \end{Bmatrix} \\
&+ \begin{Bmatrix} \left(1-\delta_{i,\frac{n}{2}+1}\right) \begin{Bmatrix} -I_{j\leqslant i}|G_{i,i+1,i-j+1}\rangle \\ -I_{j>i}|G_{i,i+1,n+i-j+1}\rangle \end{Bmatrix} \\ \delta_{i,\frac{n}{2}+1}I_{1<j<\frac{n}{2}+1}(1-\delta_{n,4}\delta_{j,2})|G_{i,2,n-j+2}\rangle \end{Bmatrix} \\
&+ \begin{Bmatrix} \left[1-\delta_{j,n}-\delta_{i,\frac{n}{2}+1}-\delta_{i,2}\left(\delta_{j,1}+\delta_{j,2}+I_{j\geqslant\frac{n}{2}+1}\right)\right]|G_{i+1,2,j+1}\rangle \\ \delta_{j,n}|G_{i+1,2,1}\rangle \\ -\delta_{i,\frac{n}{2}+1}I_{1<j<\frac{n}{2}+1}\left|G_{\frac{n}{2},\frac{n}{2}+1,\frac{n}{2}+j}\right\rangle \\ -\delta_{i,2} \begin{Bmatrix} \delta_{j,2}|G_{i+1,2,1}\rangle \\ I_{\frac{n}{2}+1<j<n}|G_{i+1,2,n+i-j+1}\rangle \end{Bmatrix} \end{Bmatrix} \\
&- t_\perp\cdot \begin{Bmatrix} I_{1<j<i}|H_{j,j,n-i+j+1}\rangle \\ 4\delta_{i,j}|H_{j,j,1}\rangle \\ (I_{i<j<n-i+2}+2\delta_{j,n-i+2})|H_{i,i,n-j+i+1}\rangle \\ I_{j>n-i+2}|H_{n-j+2,n-j+2,n+i-j+1}\rangle \end{Bmatrix} \\
&+ t_\perp\cdot \begin{Bmatrix} (I_{1<j<i}+4\delta_{j,i})|J_{j,1,i}\rangle \\ (1-\delta_{j,i})(I_{i<j<n-i+2}+2\delta_{j,n-i+2})|J_{i,1,j}\rangle \\ I_{j>n-i+2}|J_{n-j+2,1,n-i+2}\rangle \end{Bmatrix}.
\end{aligned}
$$

$$
\begin{aligned}
\hat{H}|E_{i,j}\rangle = {} & u|E_{i,j}\rangle - 4\delta_{j,i+1}\left[(1+\delta_{i,1})|B_i\rangle + \left(1+\delta_{i,\frac{n}{2}}\right)|B_j\rangle\right] \\
&- t_\perp(1-\delta_{i,1})\cdot\left[|D_{i,j}\rangle + \begin{Bmatrix} I_{j\leqslant\frac{n}{2}+1}|D_{j,i}\rangle \\ I_{\frac{n}{2}+1<j<n-i+2}|D_{n-j+2,n-i+2}\rangle \end{Bmatrix}\right] \\
&- \begin{Bmatrix} \left[1-\delta_{i,1}+\delta_{i,2}\left(\delta_{j,\frac{n}{2}+1}-I_{j>\frac{n}{2}+1}\right)\right]|E_{i-1,j}\rangle \\ \delta_{i,2}I_{j>\frac{n}{2}+1}|E_{i-1,n-j+2}\rangle \\ \delta_{i,1}\left(1+\delta_{j,2}-\delta_{j,\frac{n}{2}+1}\right)|E_{2,n-j+2}\rangle \end{Bmatrix} \\
&- (1-\delta_{j,i+1})|E_{i,j-1}\rangle - \left(1+\delta_{j,n-i+1}-\delta_{j,n-i+2}+\delta_{i,1}\delta_{j,\frac{n}{2}}-\delta_{i,1}\delta_{j,\frac{n}{2}+1}\right)|E_{i,j+1}\rangle \\
&- (1-\delta_{j,i+1})(1+\delta_{j,n-i+1}-\delta_{j,n-i+2})|E_{i+1,j}\rangle \\
&+ t_\perp(1-\delta_{i,1})\cdot \begin{Bmatrix} -I_{j\leqslant\frac{n+i+1}{2}}|G_{i,j,1}\rangle \\ I_{j>\frac{n+i+1}{2}}|G_{i,n-j+i+1,i}\rangle \end{Bmatrix} \\
&+ t_\perp(1-\delta_{i,1}-\delta_{j,n-i+2})\cdot \begin{Bmatrix} I_{j\leqslant\frac{n}{2}+1}\cdot \begin{Bmatrix} I_{j<2i-1}|G_{j,j-i+1,j}\rangle \\ -I_{j\geqslant 2i-1}|G_{j,i,1}\rangle \end{Bmatrix} \\ I_{j>\frac{n}{2}+1}\cdot \begin{Bmatrix} -I_{j\leqslant 2i-1}|G_{n-j+2,n-i+2,1}\rangle \\ I_{j>2i-1}|G_{n-j+2,n-j+i+1,n-j+2}\rangle \end{Bmatrix} \end{Bmatrix}
\end{aligned}
$$

$$+ \ (1+\delta_{j,i+1}) \cdot \left\{ \begin{array}{l} I_{i>2}|H_{i-1,n-j+i+1,i}\rangle \\ \delta_{i,2}|H_{1,2,n-j+i+1}\rangle \\ \delta_{i,1} \cdot \left\{ \begin{array}{l} 2\delta_{j,2}|H_{2,2,1}\rangle \\ I_{\frac{n}{2}+1>j>1}|H_{2,2,n-j+3}\rangle \end{array} \right\} \end{array} \right\} + [1+\delta_{j,i+1}(1+2\delta_{i,1})]|H_{i,2,j}\rangle$$

$$+ \left\{ \begin{array}{l} I_{i>1}(1+\delta_{j,i+1})(1+\delta_{j,n-i+1}-\delta_{j,n-i+2})|H_{i,n-j+i+1,i+1}\rangle \\ \delta_{i,1}\left(1+\delta_{j,i+1}-\delta_{j,\frac{n}{2}+1}\right)|H_{1,2,n-j+i+1}\rangle \end{array} \right\}$$

$$+ \ (1+\delta_{j,i+1})(1+\delta_{j,n-i+1}-\delta_{j,n-i+2})|H_{i+1,2,j+1}\rangle.$$

The last four equations devoted to the base vectors $|F_{i,j,k}\rangle$, $|G_{i,j,k}\rangle$, $|H_{i,j,k}\rangle$, $|J_{i,j,k}\rangle$ (not containing doubly occupied sites) can be found in [58].

## Appendix B. Exemplification for ground-state wavefunctions

We present below the leading terms of explicit ground-state wavefunctions deduced for $N = 28$, at $|U/t_{\|}| = 3$. The ground state $|\Psi_g\rangle$ is normalized to unity, and contains orthonormalized basis wave vectors.

For $t_{\perp}/t_{\|} = 0.8$ one obtains for the ground-state wavefunction

$$\begin{aligned} |\Psi_g\rangle = {} & 0.181\,883|E_{7,8}\rangle + 0.181\,878|C_{7,8}\rangle + 0.175\,769|D_{7,7}\rangle + 0.169\,247|C_{6,7}\rangle \\ & + 0.169\,246|E_{6,7}\rangle + 0.157\,289|D_{6,6}\rangle + 0.145\,021|C_{5,6}\rangle + 0.145\,004|E_{5,6}\rangle \\ & + 0.138\,346|D_{8,7}\rangle + 0.138\,346|D_{7,8}\rangle + 0.128\,723|D_{6,7}\rangle + 0.128\,721|D_{7,6}\rangle \\ & + 0.128\,23|D_{5,5}\rangle + 0.111\,346|C_{4,5}\rangle + 0.111\,315|E_{4,5}\rangle + 0.110\,256|D_{5,6}\rangle \\ & + 0.110\,239|D_{6,5}\rangle + 0.101\,77|E_{6,8}\rangle + 0.101\,761|C_{6,8}\rangle + 0.097\,877|G_{7,8,1}\rangle \\ & - 0.097\,8768|G_{8,2,8}\rangle + 0.093\,1102|D_{7,9}\rangle + 0.091\,3856|D_{4,4}\rangle - 0.091\,0721|G_{7,2,7}\rangle \\ & + 0.091\,0714|G_{6,7,1}\rangle + 0.090\,9671|C_{5,7}\rangle + 0.090\,9645|E_{5,7}\rangle + 0.089\,8481|D_{8,6}\rangle \\ & + 0.089\,8458|D_{6,8}\rangle + 0.084\,5566|D_{4,5}\rangle + 0.084\,4776|D_{5,4}\rangle + 0.080\,2931|D_{5,7}\rangle + \cdots, \end{aligned} \tag{B.1}$$

while for $t_{\perp}/t_{\|} = 0.1$ one has

$$\begin{aligned} |\Psi_g\rangle = {} & 0.298\,66|E_{7,8}\rangle + 0.293\,65|E_{6,7}\rangle + 0.284\,039|E_{5,6}\rangle + 0.270\,726|E_{4,5}\rangle \\ & + 0.255\,311|E_{3,4}\rangle + 0.240\,496|E_{2,3}\rangle + 0.230\,556|E_{1,2}\rangle + 0.166\,58|C_{7,8}\rangle \\ & + 0.156\,952|C_{6,7}\rangle + 0.149\,053|E_{6,8}\rangle + 0.145\,317|E_{5,7}\rangle + 0.139\,42|E_{4,6}\rangle \\ & + 0.137\,923|C_{5,6}\rangle + 0.131\,927|E_{3,5}\rangle + 0.123\,835|E_{2,4}\rangle + 0.116\,908|E_{1,3}\rangle \\ & + 0.110\,056|C_{4,5}\rangle + 0.081\,715|C_{6,8}\rangle + 0.075\,5983|E_{6,9}\rangle + 0.075\,1106|H_{6,13,7}\rangle \\ & - 0.075\,0843|H_{7,2,9}\rangle + 0.074\,6358|C_{3,4}\rangle + 0.074\,4796|C_{5,7}\rangle + 0.074\,3108|E_{5,8}\rangle \\ & + 0.074\,0908|B_7\rangle - 0.073\,841|H_{5,13,6}\rangle - 0.073\,8214|H_{6,2,8}\rangle - 0.072\,2444|B_6\rangle \\ & + 0.071\,8117|E_{4,7}\rangle - 0.071\,3933|H_{5,2,7}\rangle - 0.071\,3921|H_{4,13,5}\rangle + 0.069\,3442|B_5\rangle \\ & + \cdots \end{aligned} \tag{B.2}$$

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