Finite-Energy Pseudoparticle Theory for the 1D Hubbard Model II: Holon and Spinon Dominant Processes for the Few-Electron Spectral Weight Properties

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In the first paper of this series it was found that the $\eta$-spin 1/2 holons, spin 1/2 spinons, and $c$ pseudoparticles whose occupancy configurations describe the energy eigenstates of the one-dimensional Hubbard model emerge from the electron - rotated-electron unitary transformation. An important breakthrough is that the theory provides relevant information about the relationship of the original electrons to these quantum objects. In this second paper we discuss and clarify how such a relation can be used in a program for evaluation of finite-energy few-electron spectral functions. As a first step, here we characterize the dominant holon and spinon microscopic physical processes that originate more than 99% of the few-electron spectral weight. These dominant processes are related to exact selection rules for the values of the number of holons and spinons generated or annihilated by application onto a ground state of rotated-electron operators. While our theory also describes the higher-order microscopic processes associated with the remaining less than 1% few-electron spectral weight, the clarification and study of the above dominant processes is valuable and useful for the further understanding and description of the few-electron spectral properties observed in real low-dimensional materials. Moreover, in this paper generalize the concepts of a lower Hubbard band and upper Hubbard bands to all values of on-site Coulombian repulsion.

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I. INTRODUCTION

In this paper and its two companion papers [1, 2] the relation of the electrons of the one-dimensional (1D) Hubbard model to the quantum objects whose occupancy configurations describe its energy eigenstates is investigated for the whole Hilbert space. The study of such a non-perturbative relation is a necessary step for the description of the finite-energy few-electron spectral properties of the many-electron quantum problem.

The study of the one-dimensional (1D) Hubbard model [3, 4, 5, 6, 7, 8, 9] for interacting electrons is of general importance because the understanding of correlated systems and of their finite-energy excitations is still far from complete. The problem of the 1D Hubbard model in the limit of large and infinite on-site Coulomb repulsion was previously studied in the literature by many authors [10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22]. Our studies of the model for finite values of the on-site repulsion $U$ are motivated by the anomalous one-electron and two-electron spectral properties observed in metallic and insulating phases of quasi-one-dimensional materials, which cannot be described by the usual Fermi-liquid theory [23, 24]. Recently there has been a renewed experimental interest on the properties of these materials [25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45]. Some of these experimental studies observed unusual finite-energy/frequency spectral properties [28, 29, 30, 31]. Since in the case of finite-excitation energy the Luttinger liquid description does not apply [46, 47, 48], these finite-energy/frequency spectral properties are far from being well understood. However, there are indications that electronic correlation effects might play an important role in the finite-energy physics of these low-dimensional materials [28, 29, 30, 31, 41]. For low values of the excitation energy the microscopic electronic properties of these materials are usually described by systems of coupled chains. On the other hand, for finite values of the excitation energy larger than the transfer integrals for electron hopping between the chains, 1D lattice models taking into account the screened electron-electron Coulomb repulsion are expected to provide a good description of the physics of these materials. The simplest of these models is the above 1D Hubbard model [3, 4, 5, 6, 7, 8, 9], which describes such electron-electron interactions by an effective on-site Coulomb repulsion $U$. This model corresponds to a non-perturbative electronic problem. According to the results of the companion paper [1], its energy eigenstates can be described by occupancy configurations of holons, spinons, and $c$ pseudoparticles. Holons and spinons has also been studied for other models [49, 50, 51, 52]. The 1D Hubbard model is often considered a suitable model for the description of the electronic correlation effects and the non-perturbative microscopic mechanisms behind the unusual few-electron spectral properties observed in quasi-one-dimensional materials [28, 29, 41, 44]. Moreover, recent angle-resolved ultraviolet photoemission spectroscopy revealed very similar spectral fingerprints from both high-$T_c$ superconductors and quasi-one-dimensional compounds [26]. The similarity of the ultraviolet data for these two different systems could be evidence of the occurrence of a
charge-spin separation associated with holons and spinons. The anomalous temperature dependence of the spectral function could also indicate a dimensional crossover\cite{26, 53, 54, 55}. The results of Refs.\cite{56, 57} also suggest that the unconventional spectral properties observed in two-dimensional (2D) materials could have a 1D origin. Thus the holons and spinons could play an important role in spectral properties of both 1D and 2D low-dimensional materials.

In this second paper we continue the studies of the first paper of this series, Ref.\cite{1}. As a preliminary application of the connection of the concept of rotated electron to the quantum numbers that label the energy eigenstates provided by the Bethe-ansatz solution and \( \eta \)-spin and spin symmetries, in this paper we use exact holon and spinon selection rules for rotated-electron operators in the study of the holon and spinon contents of few-electron excitations. This reveals the dominant holon and spinon microscopic physical processes that generate more than 99\% of the spectral weight of few-electron excitations. While our theory also describes the higher-order processes associated with the remaining less than 1\% electronic spectral weight, the clarification of the dominant holon and spinon microscopic mechanisms is valuable for the further understanding and description of the few-electron spectral properties observed in real low-dimensional materials. Fortunately, a preliminary application of the theoretical predictions which follow from our study of the holon and spinon contents of few-electron excitations leads to quantitative agreement with the charge and spin spectral branch lines observed by means of angle-resolved photoelectron spectroscopy (ARPES) in the organic conductor TTF-TCNQ\cite{58}. The preliminary results reported in Ref.\cite{58} confirm that from the experimental point of view only the spectral weight associated with the dominant holon and spinon microscopic processes is observed. Moreover, in this paper we introduce the concept of an effective electronic lattice. The expression of the electrons in terms of holons, spinons, and pseudoparticles through the electron - rotated-electron transformation studied here for all values of \( U \) is a first necessary step for the evaluation of finite-energy few-electron spectral function expressions, as further discussed in Sec.\ V.

In this paper we also discuss and clarify how the relationship of the original electrons to the quantum objects whose occupancy configurations describe the energy eigenstates can be used in a program for evaluation of finite-energy few-electron spectral functions. The successful fulfilment of such a program needs the concepts of local pseudoparticle and effective pseudoparticle lattice introduced in the third paper of this series,\cite{2}. Moreover, in this paper we generalize the concepts of a lower Hubbard band and upper Hubbard bands to all values of on-site Coulombian repulsion.

The paper is organized as follows: In Sec.\ II we provide a short introduction to the 1D Hubbard model. The definition of the upper Hubbard bands in terms of rotated-electron double occupation, the holon and spinon selection rules for rotated-electron operators, and the concept of an effective electronic lattice are presented and introduced in Sec.\ III. The dominant holon and spinon microscopic physical processes that control the few-electron spectral properties are studied in Sec.\ IV. Finally, in Sec.\ V we present the discussion of our results and the concluding remarks. This includes the discussion of the application of the concepts introduced in the present series of three papers to the fulfilment of a program for evaluation of finite-energy few-electron spectral functions.

\section{II. THE 1D HUBBARD MODEL}

In a chemical potential \( \mu \) and magnetic field \( H \) the 1D Hubbard Hamiltonian can be written as,

\[
\hat{H} = \hat{H}_H - (U/2) [\hat{N} + N_a/2] + \sum_{\alpha=c, s} \mu_\alpha \hat{S}_z^\alpha
\]

(1)

where,

\[
\hat{H}_H = T + U \hat{D},
\]

(2)

is the "simple" Hubbard model. The operators

\[
\hat{T} = -t \sum_{j=1}^{N_a} \sum_{\sigma=\uparrow, \downarrow} \sum_{\delta=-1, +1} c_{j, \sigma}^\dagger c_{j+\delta, \sigma},
\]

(3)

and

\[
\hat{D} = \sum_{j=1}^{N_a} \hat{n}_{j, \uparrow} \hat{n}_{j, \downarrow},
\]

(4)
The electron number operator reads $\hat{N}_\sigma = \sum_j \hat{n}_{j,\sigma}$, (6)

counts the number of spin $\sigma$ electrons. The momentum operator reads

$$\hat{P} = -\frac{i}{2} \sum_{\sigma} \sum_{j=1}^{N_a} \left[ \hat{c}_{j,\sigma} \hat{c}_{j+1,\sigma} - \hat{c}_{j+1,\sigma} \hat{c}_{j,\sigma} \right],$$

and commutes with the Hamiltonian introduced in Eq. (1).

There are $N_\uparrow$ spin-up electrons and $N_\downarrow$ spin-down electrons in the chain of $N_a$ sites, lattice constant $a$, and length $L = [N_a a]$ associated with the model (1). We introduce Fermi momenta which in the present thermodynamic limit $L \rightarrow \infty$ are given by $\pm k_{F\uparrow} = \pm \pi n_\uparrow$ and $\pm k_F = \pm [k_{F\uparrow} + k_{F\downarrow}]/2 = \pm \pi n/L$, where $n_\sigma = N_\sigma/L$ and $n = N/L$. The electronic density can be written as $n = n_\uparrow + n_\downarrow$ and the spin density is given by $m = n_\uparrow - n_\downarrow$. In general we consider densities in the domains $0 \leq n \leq 1/a$; $1/a \leq n \leq 2/a$ and $-n \leq m \leq n$; $-(2/a-n) \leq m \leq (2/a-n)$, respectively. However, in the case of the study of transitions whose initial state is a ground state, for simplicity we restrict our considerations to values of the electronic density $n$ and spin density $m$ such that $0 \leq n \leq 1/a$ and $0 \leq m \leq n$, respectively. The Hamiltonian $\hat{H}_{SO(4)} \equiv \hat{H} - (U/2) [\hat{N} + N_a/2]$ commutes with the six generators of the $\eta$ spin $S_\eta$ and spin $S_\sigma$ algebras [3, 4, 59], respectively.

As in the first paper of this series [1], here we denote the holons (and spinons) according to their $\eta$-spin projections $\pm 1/2$ (spin projections $\pm 1/2$). For the definition of the holon and spinon numbers, their relations, and other aspects of the holon, spinon, and pseudoparticle description which are useful for the studies of this paper see the companion paper [1]. An important concept introduced in Ref. [3] is that of CPHS ensemble subspace where CPHS stands for c pseudoparticle, holon, and spinon. This is a Hilbert subspace spanned by all states with fixed values for the $-1/2$ Yang holon number $L_\gamma_{-1/2}$, $-1/2$ HL spinon number $L_\alpha_{-1/2}$, c pseudoparticle number $N_c$, and for the sets of $\alpha, \nu$ pseudoparticle numbers $\{N_{c,\nu}\}$ and $\{N_{\nu}\}$ corresponding to the $\nu = 1, 2, 3, \ldots$ branches. We note that according to the notation of Ref. [1] in HL spinon HL stands for Heilmann and Lieb.

III. THE UPPER HUBBARD BANDS, SELECTION RULES FOR ROTATED-ELECTRON OPERATORS, AND THE EFFECTIVE ELECTRONIC LATTICE

In this section we generalize the large-$U$ concept of upper Hubbard band [12] to all values of the on-site electronic repulsion $U$ in terms of rotated-electron double occupation. Moreover, we use the relation of rotated electrons to holons and spinons to introduce rotated-electron exact selection rules. These rules limit the values of the deviations in holon and spinon numbers associated with excited states generated by application of rotated-electron operators onto any eigenstate of the electronic spin $\sigma$ number operator (19). Deviation values outside the ranges given by these selection rules correspond to forbidden excited states. In addition, in this section we introduce the concept of an effective electronic lattice. This concept is further used in the third paper of this series, Ref. [2], in the introduction of the concepts of a local pseudoparticle and an effective pseudoparticle lattice. The latter concepts play an important role in the studies of finite-energy few-electron spectral functions of Refs. [60, 61].
A. ROTATED ELECTRONS AND THE UPPER HUBBARD BANDS

As discussed in the companion paper [1], the operator $c_{j,\sigma}^\dagger$ represents the rotated electrons. The relation of such an operator to the electronic operator $c_{j,\sigma}^\dagger$ is such that,

$$c_{j,\sigma}^\dagger = \hat{V}(U/t) \tilde{c}_{j,\sigma}^\dagger \hat{V}(U/t).$$

(8)

Here $\hat{V}(U/t)$ is the electron - rotated-electron unitary operator uniquely defined by Eqs. (43)-(45) of Ref. [1]. The rotated-electron double-occupation operator plays an important role in our studies and is given by,

$$\hat{D} \equiv \hat{V}(U/t) \hat{D} \hat{V}(U/t) = \sum_j \tilde{c}_{j,\uparrow}^\dagger \tilde{c}_{j,\downarrow}^\dagger \tilde{c}_{j,\downarrow} \tilde{c}_{j,\uparrow},$$

(9)

where $\hat{D}$ is the electron double occupation operator given in Eq. [1]. Note that $c_{j,\sigma}^\dagger$ and $\tilde{c}_{j,\sigma}^\dagger$ are only identical in the $U/t \rightarrow \infty$ limit where electron double occupation becomes a good quantum number.

Let the operator $\hat{O}_N(k)$ (or $\hat{D}_N(k)$) have momentum $k$ and be a product of a finite number

$$\mathcal{N} = \sum_{l_c, l_s = \pm 1} \mathcal{N}_{l_c, l_s},$$

(10)

of one-electron (or one-rotated-electron) elementary creation and/or annihilation operators. Here the ratio $\mathcal{N}/N_a$ vanishes in the present thermodynamic limit and $\mathcal{N}_{l_c, l_s}$ is the number of electron (or rotated-electron) creation and annihilation operators for $l_c = -1$ and $l_c = +1$, respectively, and with spin down and spin up for $l_s = -1$ and $l_s = +1$, respectively.

The studies we present below in this paper refer to the transformations generated by the application of the general $\mathcal{N}$-electron operator $\hat{O}_N(k)$ (or $\mathcal{N}$-rotated-electron operator $\hat{D}_N(k)$) onto any eigenstate of the spin $\sigma$ electron number operator [10]. However, we focus our attention on the particular case of states $\hat{O}_N(k)|GS\rangle$ (or $\hat{D}_N(k)|GS\rangle$) which result from application of such an operator onto a ground state $|GS\rangle$. We note that the number of spin $\sigma$ electrons equals the number of spin $\sigma$ rotated electrons.

According to the results of the companion paper [1], rotated-electron double occupation equals the number of $-1/2$ holons. We emphasize that for electronic densities $n$ such that $0 < n < 1/\alpha$ the ground state has no $-1/2$ holons [1, 8]. Since rotated-electron double occupation is a good quantum number, in this case we can write a general $\mathcal{N}$-electron spectral function as follows,

$$A_N(k, \omega) = \sum_{M=0}^{\infty} A_{N, M}(k, \omega),$$

(11)

where

$$A_{N, M}(k, \omega) = \sum_j |\langle M, j|\hat{O}_N(k)|GS\rangle|^2 \delta(\omega - \omega_{M, j}),$$

(12)

the excitation energy $\omega$ is positive, the $M$ summation of Eq. [11] runs over the values of rotated-electron double occupation $M = 0, 1, 2, \ldots$ of the excited energy eigenstates $|M, j\rangle$, the $j$ summation of Eq. [12] runs over all available excited energy eigenstates $|M, j\rangle$ with the same value $M$ of rotated-electron double occupation, and $\omega_{M, j} \equiv |E_{M, j} - E_GS|$ are the excitation energies relative to the initial ground state. Examples of few-electron operators $\hat{O}_N(k)$ whose spectral-function excitation energy is usually considered positive are the one-electron spin $\sigma$ creation operator of momentum $k$, the two-electron charge operator of momentum $k$, and the two-electron singlet or triplet Cooper pair addition operator of momentum $k$.

We call lower Hubbard band the spectral weight distribution associated with the function $A_{N, 0}(k, \omega)$ defined in Eq. [12]. Moreover, we call $M$th upper Hubbard band the spectral weight distribution associated with the function $A_{N, M}(k, \omega)$ defined in Eq. [12] such that $M > 0$. In the ensuing section we find that for one-electron and two-electron operators most spectral weight correspond to the lower Hubbard band and first (or first and second) upper
Hubbard band(s). The detailed study of the few-electron spectral functions \([\text{Eq. } 11]\) is for finite values of \(U\) a complex many-electron open problem. Such a problem is studied in Ref. [61] by the combination of the pseudofermion representation introduced in Ref. [60] with the holon and spinon description introduced and studied in this paper and in its companion papers [1, 2], as discussed in Sec. V. In this paper we use the relation of electrons and rotated electrons to the quantum objects whose occupancy configurations describe the ground state and excited states \([M, j]\) that appear in Eqs. \([11]\) and \([12]\) to obtain useful information about the finite-energy few-electron spectral distributions.

An interesting property is that in the metallic phase of the 1D Hubbard model the minimum value of the excitation energy \(\omega\) for the lower Hubbard band is zero. This justifies the designation lower band. On the other hand, the minimum value of the excitation energy for the \(Mth\) upper Hubbard band is for finite values of \(U\) finite. Such a value depends on the minimum excitation-energy value for the creation of a \(-1/2\) holon. In the case of the Hamiltonian \([1]\), this minimum energy value is for electronic densities \(n\) such that \(0 \leq n \leq 1/a\) given by \(\Delta E = E_u\). For a zero spin density \(m = 0\) initial ground state, the energy \(E_u = 2\mu(U/t, n)\) equals twice the chemical potential and is an increasing function of the on-site repulsion \(U\) with the following limiting values,

\[
E_u = 4t \cos(\pi n a/2); \quad U/t \to 0 ,
= U + 4t \cos(\pi n a); \quad U/t \to \infty .
\]  

Moreover, this energy parameter for any value of \(U/t\) is a decreasing function of the electronic density \(n\) such that,

\[
E_u = U + 4t; \quad n \to 0 ,
= E_{MH}; \quad n \to 1 ,
\]  

where \(E_{MH}\) is the half-filling Mott-Hubbard gap \([3]\). On the other hand, if one uses as initial state the same \(m = 0\) ground state but considers the excitation energy of the ”simple” Hubbard Hamiltonian \([2]\), there is a shift in the definition of the ground-state zero-energy level. For this Hamiltonian the minimum excitation-energy value for creation of a \(-1/2\) holon is simply given by \(U\).

Since rotated-electron double occupation equals the number of \(-1/2\) holons, the minimum excitation-energy value for an excited energy eigenstate with rotated electron double occupation \(M' \geq 0\) is \(\Delta E = M' E_u\). This justifies why all gapless excitation branches are associated with zero rotated-electron double occupation states. The excitation energy \(\Delta E = M' E_u\) is measured from the ground-state level and corresponds to the Hamiltonian \([1]\). If instead we consider the ground-state zero-energy level associated with the Hamiltonian \([2]\), the value of such an excitation energy becomes \(M'U\).

Any operator \(\hat{O}\) can be expanded as follows,

\[
\hat{O} = \sum_{M \in \mathbb{Z}} \hat{O}_{ME_u} , \quad (15)
\]

where \(M = \ldots -3, -2, -1, 0, 1, 2, 3, \ldots\) is such that application of the operator \(\hat{O}_{ME_u}\) onto any eigenstate of rotated electron double occupation of eigenvalue \(M'\) leads to a final state with rotated electron double occupancy \(|M' + M| \geq 0\). Also the corresponding rotated operator \(\hat{\hat{O}}\) such that,

\[
\hat{\hat{O}} = \hat{V}^\dagger(U/t) \hat{O} \hat{V}(U/t) , \quad (16)
\]

can be decomposed as,

\[
\hat{\hat{O}} = \sum_{M \in \mathbb{Z}} \hat{\hat{O}}_{ME_u} . \quad (17)
\]

The index \(ME_u\) of expressions \([14]\) and \([16]\) plays the same role as the index \(nU\) of Ref. \([12]\). While \(M = n\), the energy \(E_u\) only equals \(U\) in the \(U/t \to \infty\) limit. Since our study refers to all values of \(U/t\), here we use \(E_u\) instead of \(U\) to label the energy of the different upper Hubbard bands defined above. For finite values of \(U/t\) the choice of Ref. \([12]\) refers to the zero-energy level of the Hamiltonian \([2]\), whereas our choice corresponds to the ground-state zero-energy level of the more suitable Hamiltonian \([1]\). Our choice is justified by the fact that in real experiments the excitation energy is, in general, measured from the Fermi level. Our notation tells that the minimal amount of excitation energy
for a transition which results from application of an operator component $\hat{O}_{ME_u}$ onto any eigenstate of rotated electron double occupation $ME_u$. This excitation energy can be positive ($M > 0$) or negative ($M < 0$). We note that application onto a state of rotated-electron double occupation $M' < |M|$ of a $M < 0$ operator component $\hat{O}_{ME_u}$ gives zero. Since for the present case of electronic densities $n$ such that $0 \leq n \leq 1/a$, the ground state has zero rotated-electron double occupation, all the final excited states of the general $\bar{N}$-electron spectral function \[11\]-\[12\] have $M \geq 0$.

The operators $\hat{V}^\dagger(U/t)$ and $\hat{V}(U/t)$ associated with the electron - rotated-electron unitary transformation can be written as,

$$\hat{V}^\dagger(U/t) = e^{-\hat{S}}; \quad \hat{V}(U/t) = e^{\hat{S}}.$$  \tag{18}

These operators are uniquely defined by Eqs. (44) and (45) of the companion paper \[1\] and can be expressed in the form of an expansion in $t/U$ for the operator $\hat{S}$ \[11\]. An important role in such an expansion is played by the rotated kinetic energy operator $\hat{T}$, associated with the operator $\hat{S}$. The decomposition \[17\] of this operator leads to three terms,

$$\hat{T} = \hat{T}_0 + \hat{T}_{E_u} + \hat{T}_{-E_u}, \tag{19}$$

where

$$\hat{T}_0 = -t \sum_{j=1}^{N_u} \sum_{\sigma = \uparrow, \downarrow} \sum_{\delta = -1, +1} \left[ (1 - \hat{n}_{j, \sigma}) \hat{c}_{j, \sigma}^\dagger \hat{c}_{j+\delta, \sigma} (1 - \hat{n}_{j+\delta, \sigma}) \right. \left. + \hat{n}_{j, \sigma} \hat{c}_{j, \sigma}^\dagger \hat{c}_{j+\delta, \sigma} \hat{n}_{j+\delta, \sigma} \right], \tag{20}$$

$$\hat{T}_{E_u} = -t \sum_{j=1}^{N_u} \sum_{\sigma = \uparrow, \downarrow} \sum_{\delta = -1, +1} \hat{n}_{j, \sigma} \hat{c}_{j, \sigma}^\dagger \hat{c}_{j+\delta, \sigma} (1 - \hat{n}_{j+\delta, \sigma}), \tag{21}$$

and

$$\hat{T}_{-E_u} = -t \sum_{j=1}^{N_u} \sum_{\sigma = \uparrow, \downarrow} \sum_{\delta = -1, +1} (1 - \hat{n}_{j, \sigma}) \hat{c}_{j, \sigma}^\dagger \hat{c}_{j+\delta, \sigma} \hat{n}_{j+\delta, \sigma}. \tag{22}$$

In these expressions $\hat{\sigma}$ is such that $\hat{\uparrow} = \downarrow$ and $\hat{\downarrow} = \uparrow$. The above-mentioned expansion of the operator $\hat{S}$ of the expressions of Eq. \[18\] in powers of $t/U$ is obtained by systematic use of Eqs. (44) and (45) of the companion paper \[1\], with the result,

$$\hat{S} = \frac{1}{U} \left( \hat{T}_{E_u} - \hat{T}_{-E_u} \right) + \frac{1}{U^2} \left[ \hat{T}_{E_u} + \hat{T}_{-E_u}, \hat{T}_0 \right] + ..., \tag{23}$$

where the components of the rotated kinetic energy operator are given in Eqs. \[20\]-\[22\]. While equations (44) and (45) of Ref. \[1\] uniquely define the electron - rotated-electron unitary operator $\hat{V}(U/t)$ of Eq. \[18\] for all values of $U/t$, it is difficult to extract a closed form expression for that operator from these equations.

Let us consider the case of few-electron operators $\hat{O}_N(k)$ whose spectral-function excitation energy is usually considered negative. Example of such operators are the one-electron spin $\sigma$ annihilation operator of momentum $k$ and the two-electron singlet or triplet Cooper pair annihilation operator of momentum $k$. We note that according to the results of the companion paper \[1\], the number of rotated-electron empty sites equals the number $M_{c+1/2}$ of $+1/2$ holons. According to Eq. (C24) of the same paper, for values of the electronic density $n$ such that $0 \leq n \leq 1/a$ the ground state has a number of $+1/2$ holons whose value is given by $M^0_{c+1/2} = |N_u - \bar{N}|$. Since the number of rotated-electron empty sites is a good quantum number, we can write a general $\bar{N}$-electron spectral function associated with such a type of few-electron operators as follows,

$$B_N(k, \omega) = \sum_{M=0, \pm1, \pm2, ...}^\pm\infty B_{N,M}(k, \omega), \tag{24}$$
where

\[ B_{N,M}(k, \omega) = \sum_j |\langle M, j | \hat{O}_{N}(k) | GS \rangle|^2 \delta(\omega + \omega_{M,j}), \]  

(25)

the excitation energy \( \omega \) is negative, the \( M = [M_{c,+2} - M_{c,+2}] \) summation of Eq. 24 runs over the values of the deviation in the number of rotated-electron empty sites \( M = 0, \pm 1, \pm 2, \ldots, \pm \infty \) of the excited energy eigenstates \( |M, j\rangle \), the \( j \) summation of Eq. 25 runs over all available excited energy eigenstates \( |M, j\rangle \) with the same value \( M_{c,+2} = [M_{c,+2} + M] \) for the number of rotated-electron empty sites, and \( \omega_{M,j} = |E_{M,j} - E_{GS}| \) are the excitation energies relative to the initial ground state. Note that in the case of half filling the ground-state value for the number of rotated-electron empty sites is zero and the \( M \) summation of Eq. 24 runs over positive values of rotated-electron empty sites \( M = 0, 1, 2, \ldots, \infty \) only. Moreover, for electronic densities \( n > 1/2 \) the role of the numbers of rotated-electron doubly occupied and empty sites is interchanged. For these densities the summations over the values of rotated-electron doubly occupied and empty sites of Eqs. 11 and 24, respectively, correspond to both positive and negative integers and to positive integers, respectively. This is because for such densities the ground state has no \(+1/2\) holons. In this paper we consider mostly the case of electronic densities \( n < 1/2 \), where the ground state has no \(-1/2\) holons.

As further discussed in Sec. V, the first step for the evaluation of the general few-electron spectral functions 11-12 and 24-25 is the expression of the \( \hat{N} \)-electron operator \( \hat{O}_{N}(k) \) in terms of the corresponding rotated operator \( \hat{O}_{N}(k) \) defined in Eq. 10 as follows 61,

\[ \hat{O}_{N}(k) = \hat{V}(U/t) \hat{O}_{N}(k) \hat{V}^\dagger(U/t) \]

\[ = \hat{O}_{N}(k) + \{\hat{S}, \hat{O}_{N}(k)\} + \frac{1}{2} \{\hat{S}, [\hat{S}, \hat{O}_{N}(k)]\} + \ldots. \]  

(26)

According to the results of the companion papers 1,2, the relation of the rotated operators on the right-hand side of Eq. 26 to the quantum objects whose occupancy configurations describe the ground state and excited states \( |M, j\rangle \) and \( |M, j\rangle \) of the few-electron spectral functions 11-12 and 24-25, respectively, is well defined. Expression of the second expression of Eq. 26 in terms of the creation and annihilation operators for these quantum objects plays a crucial role in the evaluation of the matrix elements of the few-electron spectral functions 12 and 25. This justifies the importance of the holon, spinon, and c pseudoparticle description introduced in the companion paper 1 and further studied here and in the companion paper 2 for the study of the few-electron spectral properties at finite values of the excitation energy. Solution of this problem is a direct application of the relation of rotated electrons to the quantum numbers of the Bethe-ansatz solution and \( \eta \)-spin and spin symmetries found in the companion paper 1. Such a breakthrough provided the relation of electrons and rotated electrons to the above-mentioned quantum objects.

In the ensuing section we find that the first operator term of the second expression on the right-hand side of Eq. 26 corresponds to the dominant microscopic physical processes that control the few-electron spectral-weight properties. In the case of \( \hat{N} = 1 \)-electron operators we find that more than 99% of the electronic spectral weight generated by application of the operator \( \hat{O}_{N} \) onto a ground state corresponds to application of the corresponding \( \hat{N} \)-rotated-electron operator \( \hat{O}_{N} \) onto the same state. This latter operator has a simple expression in terms of holon and spinon elementary operators, and it is associated with the dominant holon and spinon microscopic mechanisms that control the \( \hat{N} \)-electron spectral properties.

**B. EXACT HOLON, SPINON, AND c PSEUDOPARTICLE SELECTION RULES FOR ROTATED-ELECTRON OPERATORS**

Let \( |\phi\rangle \) be any eigenstate of the spin \( \sigma \) electron number operator 6 and \( \hat{O}_{N} \) (or \( \hat{O}_{N} \)) a general \( \hat{N} \)-electron (or \( \hat{N} \)-rotated-electron) operator. The corresponding state \( \hat{O}_{N}|\phi\rangle \) (or \( \hat{O}_{N}|\phi\rangle \)) is also an eigenstate of the spin \( \sigma \) electron number operator 6. Such a state belongs to an electron ensemble space whose electron numbers differ from the numbers of the initial state by deviations \( \Delta N_\uparrow \) and \( \Delta N_\downarrow \), such that \( \Delta N = \Delta N_\uparrow + \Delta N_\downarrow \). Since the number of spin \( \sigma \) electrons equals the number of spin \( \sigma \) rotated electrons, these deviations also refer to the latter numbers. These deviations can be expressed in terms of the numbers \( N_{l,\uparrow} \) of Eq. 10 as follows,

\[ \Delta N_\uparrow = \sum_{l_\uparrow = \pm 1} (-l_\uparrow) N_{l_\uparrow, +1}; \quad \Delta N_\downarrow = \sum_{l_\downarrow = \pm 1} (-l_\downarrow) N_{l_\downarrow, -1}. \]  

(27)
Following the results of Refs. [1, 8], let us consider the four expectation values $R_{\alpha, l_\alpha} = \langle \hat{R}_{\alpha, l_\alpha} \rangle$, where $\alpha = c, s$ and $l_\alpha = -1, +1$ and the corresponding operator $\hat{R}_{c, -1}$ counts the number of electron doubly-occupied sites, $\hat{R}_{c, +1}$ counts the number of electron empty sites, $\hat{R}_{s, -1}$ counts the number of spin-down electron singly-occupied sites, and $\hat{R}_{s, +1}$ counts the number of spin-up electron singly-occupied sites. These operators are given in Eqs. (23) and (24) of the companion paper [1]. In reference [8] it was found that in the limit $U/t \to \infty$ the deviations $\Delta R_{c, -1}$, $\Delta R_{c, +1}$, $\Delta R_{s, -1}$, and $\Delta R_{s, +1}$ generated by application of a general $N$-electron operator $\hat{O}_N$ onto any eigenstate of the spin $\sigma$ electron number operator $O$ are restricted to the ranges of the inequalities (60)-(63) of the same reference. Obviously, given one of the four ranges of values defined by these four inequalities, the other three are dependent and follow from the relations given in Eq. (56) of Ref. [8].

Let us consider the deviations $\Delta R_{c, -1}$, $\Delta R_{c, +1}$, $\Delta R_{s, -1}$, and $\Delta R_{s, +1}$ in the expectation values of the four operators given in Eqs. (23) and (24) of Ref. [1] in the case that both the corresponding initial state $|\phi_l\rangle$ and final state $|\phi_{l'}\rangle$ are energy eigenstates of the 1D Hubbard model in the limit $U/t \to \infty$. Note that it is assumed that the final energy eigenstate $|\phi_{l'}\rangle$ is contained in the state $\hat{O}_N |\phi_l\rangle$ where $\hat{O}_N$ is the general $N$-electron operator under consideration. In the case of these initial and final states the above-mentioned deviations are such that,

$$
\Delta R_{\alpha, l_\alpha} = \langle \phi_{l'} | \hat{R}_{\alpha, l_\alpha} | \phi_{l'} \rangle - \langle \phi_l | \hat{R}_{\alpha, l_\alpha} | \phi_l \rangle = 
\langle \psi_l (U/t) | \hat{V}^\dagger (U/t) \hat{R}_{\alpha, l_\alpha} \hat{V} (U/t) | \psi_{l'} (U/t) \rangle - 
\langle \psi_{l'} (U/t) | \hat{V}^\dagger (U/t) \hat{R}_{\alpha, l_\alpha} \hat{V} (U/t) | \psi_l (U/t) \rangle,
$$

for all values of $U/t$. In order to derive this result we used Eq. (52) of the companion paper [1]. Also Eqs. (54)-(57) of the same paper were used in the evaluation of the equalities on the right-hand side of Eq. (28). Equation (52) of Ref. [1] relates the energy eigenstates of the $U/t \to \infty$ Hubbard model to the corresponding energy eigenstates of the Hubbard model for any value of $U/t$. We note that the last quantity on the right-hand side of Eq. (28) is nothing but the deviation

$$
\Delta M_{\alpha, \sigma} = \langle \psi_l (U/t) | \hat{M}_{\alpha, \sigma} | \psi_l (U/t) \rangle - \langle \psi_{l'} (U/t) | \hat{M}_{\alpha, \sigma} | \psi_{l'} (U/t) \rangle = M'_{\alpha, \sigma} - M_{\alpha, \sigma},
$$

in the particular case when the initial state $|\psi_l (U/t)\rangle$ and final state $|\psi_{l'} (U/t)\rangle$ are energy eigenstates of the finite-$U/t$ Hubbard model. The final energy eigenstate $|\psi_{l'} (U/t)\rangle$ is contained in the state $\hat{O}_N |\psi_l (U/t)\rangle$, where the rotated operator $\hat{O}_N$ is related to the operator $\hat{O}_N$ by Eq. (29). The operator

$$
[\hat{O}_N - \hat{\bar{O}}_N] = [\hat{S}, \hat{\bar{O}}_N] + \frac{1}{2} [\hat{S}, [\hat{S}, \hat{\bar{O}}_N]] + ..., \tag{30}
$$

can be expressed as a sum of $N'$-electron operators such that $N' > N$. Note that Eq. (30) contains the same information as Eq. (29).

The quantities $M_{\alpha, \sigma}$ and $M'_{\alpha, \sigma}$ of Eq. (29) are the eigenvalues of the energy eigenstates $|\psi_l (U/t)\rangle$ and $|\psi_{l'} (U/t)\rangle$, respectively, relative to the holon ($\alpha = c$) or spinon ($\alpha = s$) number operator $\hat{M}_{\alpha, \sigma}$ studied in the companion paper [1]. These two states are related to the above initial state $|\phi_l\rangle$ and final state $|\phi_{l'}\rangle$ by the transformation given in Eq. (52) of the same paper. The equalities of Eq. (29) are valid for all possible $4^{N'}$ initial energy eigenstates $|\phi_l\rangle$ of the 1D Hubbard model in the limit $U/t \to \infty$ such that $l = 1, 2, ..., 4^{N'}$ and for final energy eigenstates $|\phi_{l'}\rangle$ which are contained in $\hat{O}_N |\phi_l\rangle$. According to these equalities, the deviations in the eigenvalues of the four operators $\hat{R}_{\alpha, l_\alpha}$ of Eqs. (23) and (24) of the companion paper [1] which count the number of electron doubly-occupied sites, empty sites, spin-down singly-occupied sites, and spin-up singly-occupied sites equal the deviations in the eigenvalues of the four operators $\hat{M}_{\alpha, \sigma}$ given in Eq. (22) of the same paper. These four operators count the number of $-1/2$ holons, $+1/2$ holons, $-1/2$ spinons, and $+1/2$ spinons, respectively. Note that according to Eqs. (52) and (54)-(57) of Ref. [1] such an equality is valid because the initial and final states of the latter deviations are the energy eigenstates of the finite-$U/t$ 1D Hubbard model $|\psi_l (U/t)\rangle = \hat{V}^\dagger (U/t) |\phi_l\rangle$ and $|\psi_{l'} (U/t)\rangle = \hat{V}^\dagger (U/t) |\phi_{l'}\rangle$, respectively. Here the final state $|\psi_{l'} (U/t)\rangle = \hat{V}^\dagger (U/t) |\phi_{l'}\rangle$ is contained in the state $\hat{O}_N |\psi_l (U/t)\rangle = \hat{V}^\dagger (U/t) \hat{O}_N |\phi_l\rangle$.

The electron double-occupation, no-occupation, spin-down single-occupation, and spin-up single-occupation eigenvalue deviations [28] which result from application onto the state $|\phi_l\rangle$ of the above general operator $\hat{O}_N$ are restricted to the ranges of the inequalities (60)-(63) of Ref. [8]. Therefore, also the the $-1/2$-holon-number, $+1/2$-holon-number, $-1/2$-spinon-number, and $+1/2$-spinon-number eigenvalue deviations [29] which result from application onto the state...
Interestingly, as in the \((31)-(34)\) and \((36)\). Such dominant microscopic physical processes control most of the operators at any value of \(U/t\) weight only. Moreover, for small electronic densities the dominant processes become the only processes for holes, respectively. The states with holon and spinon numbers outside the domains defined by inequalities \((31)-(34)\) and \((36)\) is maximum for half filling and at \(U\approx4t\) where it amounts for about 0.25% of the total spectral weight. Nevertheless, such a \(N\)-electron addition spectral weight for electronic densities \(n=1/a\), \(n=1/2a\), and \(n<<1/a\), respectively, as found in Sec. IV.

\[
- \sum_{l_s=\pm1} N_{+1,l_s} \leq \Delta M_{c,-1/2} \leq \sum_{l_s=\pm1} N_{-1,l_s}, \tag{31}
\]

\[
- \sum_{l_s=\pm1} N_{-1,l_s} \leq \Delta M_{c,+1/2} \leq \sum_{l_s=\pm1} N_{+1,l_s}, \tag{32}
\]

\[
- \sum_{l_c,l_s=\pm1} \delta_{l_c,-l_s} \mathcal{N}_{c,l_s} \leq \Delta M_{s,-1/2} \leq \sum_{l_c,l_s=\pm1} \delta_{l_c,-l_s} \mathcal{N}_{c,l_s}, \tag{33}
\]

and

\[
- \sum_{l_c,l_s=\pm1} \delta_{l_c,l_s} \mathcal{N}_{c,l_s} \leq \Delta M_{s,+1/2} \leq \sum_{l_c,l_s=\pm1} \delta_{l_c,l_s} \mathcal{N}_{c,l_s}. \tag{34}
\]

According to Eq. (29), the eigenvalues \(M_{\alpha,\sigma}\) and \(M'_{\alpha,\sigma}\) of these deviations refer to an initial state which is one of the \(4^N\) energy eigenstates \(|\psi(U/t)\rangle\) of the finite-\(U/t\) Hubbard model and to a final state which is an energy eigenstate \(|\psi_f(U/t)\rangle\) of the same model contained in the state \(\mathcal{O}_N|\psi(U/t)\rangle\). However, since the \(4^N\) states \(|\psi(U/t)\rangle\) associated with the deviations of Eq. \((29)\) constitute a complete basis for the Hilbert space of the 1D Hubbard model, the inequalities \((31)-(34)\) also apply to general deviations of the form,

\[
\Delta M_{\alpha,\sigma} = \langle \psi' | \hat{M}_{\alpha,\sigma} | \psi \rangle - \langle \psi | \hat{M}_{\alpha,\sigma} | \psi \rangle, \tag{35}
\]

provided that the arbitrary states \(\psi'\) and \(\psi\) are eigenstates of the spin \(\sigma\) electron number operator \(\hat{c}\).

It follows from the relations of Eq. (50) of the companion paper \([1]\) that out of the four inequalities \((31)-(34)\), only one is independent. By summation of the two inequalities \((31)\) and \((32)\) and of the two inequalities \((33)\) and \((34)\) we find the following inequalities for the deviations in the total number of holons and spinons,

\[
-N \leq \Delta N_c \leq N; \quad -N \leq \Delta N_s \leq N. \tag{36}
\]

Note that the limiting values of the inequalities \((36)\) are simply \(-N\) and \(N\), where \(N\) is the number of elementary rotated-electron operators of the expression of the operator \(\mathcal{O}_N\). Finally, through the use of Eq. (28) of Ref. \([1]\) we find that the validity of these inequalities is equivalent to the inequalities

\[
-N \leq \Delta N_c \leq N; \quad -N \leq \Delta N_s \leq N, \tag{37}
\]

for the deviations \(\Delta N_c = -\Delta N_c^h\) in the number \(N_c\) of c pseudoparticles and in the number \(N_c^h\) of c pseudoparticle holes, respectively.

We emphasize that the exact holon and spinon selection rules \((31)-(34)\) and \((36)\) refer to deviations generated by \(N\)-rotated-electron operators. We find below that in the case of deviations generated by the corresponding \(N\)-electron operator the dominant holon and spinon microscopic physical processes lead to excited states that obey the inequalities \((31)-(34)\) and \((36)\). Such dominant microscopic physical processes control most of the \(N\)-electron spectral-weight. Interestingly, as in the \(U >> t\) case, for \(U << t\) these rules are exact for the corresponding \(N\)-electron operator, the dominant processes becoming the only processes contributing to the \(N\)-electron spectral properties. On the other hand, for values of the on-site repulsion such that \(U \approx 4t\) these rules are not exact for \(N\)-electron operators but correspond to dominant processes that amount for more than 99% of the electronic spectral weight. For instance, in the case of one-electron creation operators, we find that the spectral weight generated by higher-order holon and spinon processes is extremely small. Such a weight corresponds to states with holon and spinon numbers outside the domains defined by inequalities \((31)-(34)\) and \((36)\) and is maximum for half filling and at \(U \approx 4t\) where it amounts for about 0.25% of the total spectral weight. However, such a weight decreases for decreasing values of the electronic density. For instance, at quarter filling it is maximum also for \(U \approx 4t\) but amounts for 0.005% of the total spectral weight only. Moreover, for small electronic densities the dominant processes become the only processes for \(N\)-electron operators at any value of \(U/t\). In the case of the one-electron creation operators the states generated by the dominant processes refer to a minimal amount of relative spectral weight for \(U \approx 4t\). Nevertheless, such a minimal value corresponds for the dominant holon and spinon processes to 99.75%, 99.99%, and 100.00% of the total one-electron addition spectral weight for electronic densities \(n=1/a\), \(n=1/2a\), and \(n<<1/a\), respectively, as found in Sec. IV.
C. THE EFFECTIVE ELECTRONIC LATTICE

The electron - rotated-electron unitary transformation performs a rotation in Hilbert space which maps electrons onto rotated-electrons such that rotated-electron double occupation is a good quantum number. As discussed below, the rotated-electron site distribution configurations that describe the energy eigenstates are independent on the value of the ratio $U/t$. In contrast, the electron site distribution configurations that describe these states are dependent on $U$. This is consistent with the $U/t$ dependence of the electron double-occupation quantities studied in Ref. [3].

As discussed in the companion paper [1], the electronic lattice remains invariant under the electron - rotated-electron unitary transformation. However, in order to distinguish the rotated-electron from the electronic site distribution configurations it is useful to introduce an effective electronic lattice. The rotated electrons occupy the sites of the effective electronic lattice, whereas the electrons occupy the sites of the real-space lattice. Such an effective electronic lattice has the same number of sites $j = 1, 2, 3, ..., N_\alpha$, lattice constant $a$, and length $L = N_\alpha \times a$ as the real-space lattice.

In the companion paper [2] it is found that the rotated-electron site distribution configurations that describe the energy eigenstates include separated charge and spin sequences. The charge (and spin) sequences correspond to distribution configurations of the rotated-electron doubly occupied sites and empty sites (and spin-down and spin-up singly occupied sites). For the effective electronic lattice the number of $-1/2$ holons equals rotated-electron double occupation and thus plays the same role as electron double occupation in the real-space lattice. For finite values of $U/t$, the number of electron doubly-occupied sites, empty sites, spin-down singly-occupied sites, and spin-up singly-occupied sites of the real-space lattice electron site distribution configurations that describe the energy eigenstates, is not a good quantum number. In contrast, for the effective electronic lattice the number of rotated-electron doubly-occupied sites, empty sites, spin-down singly-occupied sites, and spin-up singly-occupied sites is a good quantum number for all values of $U/t$. This number equals the number of $-1/2$ holons, $+1/2$ holons, $-1/2$ spinons, and $+1/2$ spinons, respectively, of any energy eigenstate.

A property of major importance is that the effective electronic lattice site distribution configurations of the rotated electrons which describe the energy eigenstate $|\psi(U/t)\rangle$ of the relation (52)of the companion paper [1] are the same as the corresponding real-space lattice site distribution configurations of the electrons which describe the state $|\phi\rangle$. Since this latter state is an energy eigenstate of the 1D Hubbard model in the limit $U/t \to \infty$, the rotated-electron site distribution configurations which describe the energy eigenstates are independent of the value of $U/t$ and are precisely the same as the corresponding electron site distribution configurations of the $U/t \to \infty$ 1D Hubbard model.

In the companion paper [2] it is shown that this property is behind the fact that the $c$ and $\alpha, \nu$ pseudoparticle band-momentum occupancy configurations which describe the energy eigenstates are also independent of the value of $U/t$, only the energy spectrum of such configurations are $U/t$ dependent. The fact that the $U/t \to \infty$ selection rule ranges given in Eqs. (60)-(63) of Ref. [3] are precisely the same as the finite-$U/t$ ranges imposed by the inequalities [51]-[54] results from the $U/t$ independence of the rotated-electron site distribution configurations which describe the energy eigenstates.

Another important property is that for electronic densities smaller or equal to one, a ground state has zero rotated-electron double occupation. The same occurs for the ground state electron site distribution configurations of the real-space lattice in the limit $U/t \to \infty$, the ground-state electron double occupation being in that limit given by $D^0 = R_{c,-1}^0 = 0$. This property is consistent with the above property that the rotated-electron site distribution configurations which describe the energy eigenstates are $U/t$ independent. Note that creation of a rotated electron onto the ground state either transforms an empty site of the effective electronic lattice into a singly-occupied site or a singly-occupied site of the lattice into a doubly-occupied site. These two alternative transitions lead to $-1/2$ holon number deviations such that $\Delta M_{c,-1/2} = 0$ and $\Delta M_{c,-1/2} = 1$, respectively. Therefore, the selection rule of Eq. (49) leads to permitted final states such that the values of these deviations are $\Delta M_{c,-1/2} = 0, 1$. For the effective electronic lattice the operators $\hat{M}_{c,-1/2}$, $\hat{M}_{c,+1/2}$, $\hat{M}_{s,-1/2}$, and $\hat{M}_{s,+1/2}$ count the number of rotated-electron doubly-occupied sites, empty sites, spin-down singly-occupied sites, and spin-up singly-occupied sites, respectively. Each site of the effective electronic lattice can either be doubly occupied by two rotated electrons of opposite spin projection, empty, singly occupied by a spin-down rotated electron, and singly occupied by an spin-up rotated electron. The result of Ref. [1] that the $-1/2$ holons are zero spin-singlet combinations of two electrons of opposite spin projection whereas the $+1/2$ holons are two-electronic hole quantum objects, is consistent with the $-1/2$ holons and the $+1/2$ holons corresponding to rotated-electron doubly-occupied and empty sites of the effective electronic lattice, respectively.

In the companion paper [2] it is found that the effective electronic lattice introduced here is related to a set of effective pseudoparticle lattices. The concept of effective pseudoparticle lattice introduced in that reference arises from a local description of the pseudoparticles, alternative to the band-momentum $q$ description extracted directly from the Bethe-ansatz solution in the companion paper [1]. While in the limit $U/t \to \infty$ such a local description of the pseudoparticles refers to the real-space lattice, in the case of finite values of $U/t$ the local pseudoparticle character refers to the effective electronic lattice, as discussed in Ref. [2]. In that reference the local pseudoparticles
are described in terms of rotated-electron site distribution configurations. The concepts of an effective pseudoparticle lattice and of a local pseudoparticle introduced in the companion paper \cite{2} are used in the studies of the few-electron spectral properties of the model presented in Refs. \cite{60, 61}.

IV. THE DOMINANT HOLON AND SPINON MICROSCOPIC PHYSICAL PROCESSES FOR THE FEW-ELECTRON SPECTRAL PROPERTIES

The commutation relations (60)-(62) of the companion paper \cite{1} imply that the six generators of the $\eta$-spin and spin $SU(2)$ algebras given in Eqs. (2), (9), and (10) of the same paper and the momentum operator \cite{1} have the same expressions both in terms of elementary electronic operators $c_{j,\sigma}^\dagger$ and $c_{j,\sigma}$ and elementary rotated-electron operators $\tilde{c}_{j,\sigma}$ and $\tilde{c}_{j,\sigma}$, respectively. Thus all these seven operators are both two-electron and two-rotated-electron operators. These two-electron operators are such that all operator terms of the second expression of Eq. (20) vanish except the first term. Thus the operator (30) associated with such operators vanishes. This result suggests that application of an operator of the form (30) associated with a general $N$-electron operator onto a ground state leads to very little electronic spectral weight. The latter spectral weight vanishes in the particular case that the $N$-electron operator commutes with the electron - rotated-electron unitary operator, but is expected to be extremely small otherwise, at least for few-electron operators. The reason is that such general $N$-electron and $N$-rotated-electron operators are products of the same elementary operators $c_{j,\sigma}, c_{j,\sigma}$ and $\tilde{c}_{j,\sigma}, \tilde{c}_{j,\sigma}$, respectively, as the above two-electron operators. Application of any of the above seven two-electron operators and of the corresponding two-rotated-electron operators onto a ground state leads to the same final states. Other two-electron or few-electron operators have slightly different expressions in terms of the same elementary electronic operators. Thus it is expected that the application of any other few-electron operator onto a ground state leads to almost the same final states as application of the corresponding few-rotated-electron operator on the same ground state. This is equivalent to say that application of the operator (30) associated with such operators onto a ground state leads to almost no spectral weight. This property is a direct result of the unitary and canonical character of the electron - rotated-electron transformation. This prediction is confirmed by the quantitative results obtained below. Indeed, we find that the dominant microscopic physical processes that control the $N$-electron spectral-weight distribution of the excitation $\hat{O}_N|GS\rangle$ are associated with the transformation laws of the $N$-rotated-electron operator of the second expression of Eq. (20) Indeed, in the case $N = 1$, over 99% percent of the spectral weight of $\hat{O}_N|GS\rangle$ is found to be contained in $\hat{O}_N|GS\rangle$.

We start by studying the specific form that the exact holon and spinon selection rules associated with the inequalities \cite{31, 32}, \cite{33}-\cite{36} take for transitions generated by application onto a ground state of a general $N$-rotated-electron operator. While these ground-state selection rules refer to $N$-rotated-electron operators, spectral functions of physical interest are of the form \cite{37, 38} and \cite{39}-\cite{42} and involve $N$-electron operators. Therefore, the main subject of this section is the study and discussion of the consequences of the $N$-rotated-electron ground-state selection rules on the $N$-electron spectral-weight properties. We find that the holon and spinon deviation number restrictions of the inequalities \cite{31, 32}, \cite{33}-\cite{36} correspond in the case of excitations generated by $N$-electron operators to the dominant holon and spinon microscopic physical processes that control the electronic spectral properties.

In the quantitative numerical studies presented below we devote particular attention to the basic $N = 1$ electron and rotated-electron operators. We provide evidence that the general results obtained for one-electron operators also apply to $N = 2$ and other few-electron operators.

A. THE GROUND-STATE CHARGE AND SPIN SELECTION RULES FOR ROTATED-ELECTRON OPERATORS

The inequalities \cite{31, 32}, \cite{33}-\cite{36} provide the largest domains for permitted values of $\pm 1/2$ holon and $\pm 1/2$ spinon number deviations generated by application of $N$-rotated-electron operators $\hat{O}_N$. According to Eq. (19) the number $N$ is given by $N = \sum_{l_x, l_y, l_z = \pm 1} N_{l_x, l_y, l_z}$, where the numbers $N_{-1, -1}, N_{-1, +1}, N_{+1, -1},$ and $N_{+1, +1}$ are defined below such an equation. The deviation permitted values defined by inequalities \cite{31, 32}, \cite{33}-\cite{36} are determined uniquely by the values of the four numbers $N_{l_x, l_y}$ specific to the operator $\hat{O}_N$ and do not depend on the values of $U/t$, electronic density $n$, and spin density $m$. Moreover, these inequalities provide the largest domains for permitted deviation values for all values of $U/t$, electronic densities $0 \leq n \leq 1/a$ and $1/a \leq n \leq 2/a$ and spin densities $-n \leq m \leq n$ and $-(2/a - n) \leq m \leq (2/a - n)$, respectively. However, the domains of such a permitted values can be smaller. Let $M_{\alpha, \pm 1/2}$ be the numbers of $\pm 1/2$ holons ($\alpha = c$) and $\pm 1/2$ spinons ($\alpha = s$) of the initial state. For instance, in case of deviations which do not obey the following inequalities,
\[ M_{c,-1/2}^0 \geq \sum_{l_c, l_z = \pm 1} \mathcal{N}_{l_c, l_z}, \quad M_{c,+1/2}^0 \geq \sum_{l_c = \pm 1} \mathcal{N}_{l_c, l_z}, \]
\[ M_{s,-1/2}^0 \geq \sum_{l_c, l_z = \pm 1} \delta_{l_c, l_z} \mathcal{N}_{l_c, l_z}, \quad M_{s,+1/2}^0 \geq \sum_{l_c = \pm 1} \delta_{l_c, l_z} \mathcal{N}_{l_c, l_z}, \]

(38)

the corresponding domains of deviation values are smaller and are contained in those defined by inequalities (31)-(34).

For simplicity in this section we consider initial ground states corresponding to electronic densities \(0 \leq n \leq 1/a\) and spin densities \(0 \leq m \leq n\). As discussed in the companion paper \[1\], one can generate from states with electronic densities \(0 \leq n \leq 1/a\) and spin densities \(0 \leq m \leq n\) the corresponding towers of states with electronic densities and spin densities belonging to the above extended domains. This is reached by repetitive application of the off-diagonal generators of the \(\eta\)-spin and spin algebras given in Eqs. (9) and (10) of Ref. \[1\], respectively, onto the former states.

In the particular case when the initial state is a ground state \((GS)\) with values of the density and spin density belonging to the above domains, the state \(\hat{O}_N(GS)\) belongs to an electron ensemble space with electron and rotated-electron numbers,

\[ N = N_1 + N_\downarrow = N^0 + \Delta N; \quad N_1 = N^0_1 + \Delta N_1; \quad N_\downarrow = N^0_\downarrow + \Delta N_\downarrow. \]

(39)

Here \(N^0, N^0_1\), and \(N^0_\downarrow\) are the ground-state initial electron-ensemble space electron and rotated-electron numbers and the deviations are given by the general expressions of Eq. (27). (We recall that the spin \(\sigma\) electron numbers remain invariant under the electron - rotated-electron unitary transformation and thus the number of spin \(\sigma\) electrons equals the number of spin \(\sigma\) rotated electrons.)

Let us first disregard the selection rules associated with the inequality (21). In this case the use of Eq. (24) and Eqs. (49) and (50) of the companion paper \[1\] reveals that the deviations leading to the set of final states whose \(c\)-pseudoparticle, \(-1/2\) holon, and \(-1/2\) spinon numbers are compatible with the state \(\hat{O}_N(GS)\) generated by application onto the ground state of a general \(N\)-rotated-electron operator are such that,

\[ \Delta M_{c,-1/2} = 0, 1, 2, 3, ..., N^0_\downarrow + \sum_{l_c = \pm 1} (-l_c) \mathcal{N}_{l_c, -1} = 0, 1, 2, 3, ..., N_\downarrow. \]

(40)

The corresponding possible values of the \(-1/2\) spinon number deviations \(\Delta M_{s,-1/2}\) are determined by the value of the \(-1/2\) holon number deviation \(\Delta M_{c,-1/2}\) and are given by,

\[ \Delta M_{s,-1/2} = \sum_{l_c = \pm 1} (-l_c) \mathcal{N}_{l_c, -1} - \Delta M_{c,-1/2} = \Delta N_\downarrow - \Delta M_{c,-1/2}. \]

(41)

For given initial values of the spin \(\sigma\) electron and rotated-electron numbers, only one of the two deviations \(\Delta M_{c,-1/2}\) and \(\Delta M_{s,-1/2}\) is independent. Thus Eq. (40) reveals that the number of different CPHS ensemble spaces spanned by states whose electron and rotated-electron numbers are the same as the ones of the state \(\hat{O}_N(GS)\) is \(N_\downarrow + \Delta N_\downarrow = N_\downarrow\), with \(N_\downarrow \to \infty\) in the present thermodynamic limit. This is confirmed by Eqs. (34) and (35).

According to the expressions given in Eq. (C24) of the companion paper \[1\] the number of \(-1/2\) holons vanishes in the case of a ground state and thus the inequality \(M_{c,-1/2}^0 \geq \sum_{l_c = \pm 1} \mathcal{N}_{l_c, l_z}\) given in Eq. (35) is not met except when \(\sum_{l_z = \pm 1} \mathcal{N}_{l_z} = 0\). This shortens the domain of the deviation values relative to the largest permitted domains given in inequalities (31)-(34). When the initial state is the ground state the \(-1/2\)-holon, \(+1/2\)-holon, \(-1/2\)-spinon, and \(+1/2\)-spinon number deviations are restricted to the ranges of the following inequalities,

\[ 0 \leq \Delta M_{c,-1/2} \leq \sum_{l_c = \pm 1} \mathcal{N}_{l_c, l_z}, \]

\[ \sum_{l_c, l_z = \pm 1} (l_c) \mathcal{N}_{l_c, l_z} \leq \Delta M_{c,+1/2} \leq \sum_{l_c = \pm 1} \mathcal{N}_{l_c, l_z}, \]

\[ -\sum_{l_c, l_z = \pm 1} \delta_{l_c, l_z} \mathcal{N}_{l_c, l_z} \leq \Delta M_{s,-1/2} \leq \sum_{l_c = \pm 1} (-l_c) \mathcal{N}_{l_c, -1}, \]

(42)

(43)

(44)
\begin{align}
- \sum_{l_\nu,l_\delta=\pm 1} \delta_{l_\nu,l_\delta} N_{l_\nu,l_\delta} \leq \Delta M_{c,1/2} & \leq \sum_{l_\nu=\pm 1} (-l_\nu) N_{l_\nu,1/2}. \tag{45}
\end{align}

Thus in the case of the $-1/2$ holon deviations $\Delta M_{c,-1/2}$ only the following integer values are permitted,

\begin{align}
\Delta M_{c,-1/2} = \Delta L_{c,-1/2} + \sum_{\nu=1}^{\infty} \nu \Delta N_{c,\nu} = 0, 1, 2, \ldots, \frac{N_{c,1/2}}{2}.
\end{align}

Here we used Eq. (30) of the companion paper \cite{1} to express the deviation $\Delta M_{c,-1/2}$ in terms of the deviations in the numbers of $-1/2$ Yang holons and $c, \nu$ pseudoparticles. We emphasize that the exact ground-state charge selection rule (40) also limits the value of the deviations $\Delta N^h_c$ in the number of $c$ pseudoparticle holes. Indeed such a selection rule is equivalent to the following inequality,

\begin{align}
\sum_{l_\nu,l_\delta=\pm 1} (l_\nu) N_{l_\nu,l_\delta} \leq \Delta N^h_c \leq N_e.
\end{align}

Note that this inequality is a particular case for an initial ground state of the general $\Delta N^h_c$ inequality (37).

In general the ground-state selection rule (40) also implies that the maximum permitted values of the deviations $\Delta L_{c,-1/2}$ and $\sum_{\nu=1}^{\infty} \nu \Delta N_{c,\nu}$ are $\max\{\Delta L_{c,-1/2}\} = \sum_{l_\delta=\pm 1} N_{l_\delta,1/2}$ and $\max\{\sum_{\nu=1}^{\infty} \nu \Delta N_{c,\nu}\} = \sum_{l_\nu=\pm 1} N_{l_\nu,1/2}$, respectively, provided that the condition $\max\{\Delta L_{c,-1/2} + \sum_{\nu=1}^{\infty} \nu \Delta N_{c,\nu}\} = \sum_{l_\nu=\pm 1} N_{l_\nu,1/2}$ is respected. However, we note that the value $\max\{\sum_{\nu=1}^{\infty} \nu \Delta N_{c,\nu}\} = \sum_{l_\nu=\pm 1} N_{l_\nu,1/2}$ can be reached only if the inequalities (i) $L_{c,1/2} + \sum_{l_\nu=\pm 1} N_{l_\nu,1/2} \geq \sum_{l_\nu=\pm 1} N_{l_\nu,1/2}$ and (ii) $M_{s,1/2} \geq N_{c,1/2} + M_{s,1/2} \geq N_{c,1/2}$ are met. Inequality (i) follows from the requirement that generation of a $c, \nu$ pseudoparticle involves combination of the $\nu$ new created $-1/2$ holons with a number $\nu$ of $+1/2$ holons \cite{1}. The number $L_{c,1/2}$ gives the number of these $+1/2$ holons pre-existing in the initial state and $\sum_{l_\nu=\pm 1} N_{l_\nu,1/2}$ gives the number of $+1/2$ holons created by annihilation of rotated electrons singly occupying sites in the initial state. Inequality (ii) results from two requirements: First the maximum value of $\sum_{\nu=1}^{\infty} \nu \Delta N_{c,\nu}$ is reached when each new created spin-down and/or spin-up rotated electron combines with a spin-up and/or spin-down rotated electron pre-existing in rotated-electron singly occupied sites of the initial state. This requires that $M_{s,1/2}$ be larger than or equal to $N_{c,1/2}$. Second at least $N_{c,1/2}$ of spin $\mp 1/2$ rotated electrons singly occupying sites of the initial state should be annihilated and give rise to empty sites associated with the new created $+1/2$ holons. This requires the presence of the extra term $N_{c,1/2}$ on the right-hand side of the above inequality (ii).

For instance, for the half-filling $2S^h_0 = L^h_0 = 0$ ground state the values of the $c, \nu$ pseudoparticle number deviations are restricted by the inequality $\sum_{\nu=1}^{\infty} \nu \Delta N_{c,\nu} \leq \min\{\sum_{l_\nu=\pm 1} N_{l_\nu,1/2}, \sum_{l_\nu=\pm 1} N_{l_\nu,1/2}\}$. However, there might exist other selection rules which further restrict the values of these $c, \nu$ pseudoparticle deviations. Recent numerical results \cite{67} reveal that in the case of the half-filling $2S^h_0 = L^h_0 = 0$ initial ground state, the state generated by application of the $\mathcal{N} = 2$ charge operator contains no $c, \nu$ pseudoparticles. This suggests that there is another selection rule which states that generation of $c, \nu$ pseudoparticles by new created rotated electrons results from combination of the $-1/2$ holons generated by creation of these rotated electrons with pre-existing $+1/2$ Yang holons in the initial ground state. Since for the half-filling initial ground state we have that $2S^h_0 = L^h_0 = 0$, the numerical results of Ref. \cite{67} suggest that in the case of such an initial ground state $\sum_{\nu=1}^{\infty} \nu \Delta N_{c,\nu} = 0$ and thus Eq. (40) simplifies to $\Delta M_{c,-1/2} = \Delta L_{c,-1/2} = 0, 1, 2, \ldots, \sum_{l_\nu=\pm 1} N_{l_\nu,1/2}$. Moreover, if such a selection rule is valid for all $\mathcal{N}$-rotated-electron operators, the maximum permitted value of the deviation $\sum_{\nu=1}^{\infty} \nu \Delta N_{c,\nu}$ becomes $\max\{\sum_{\nu=1}^{\infty} \nu \Delta N_{c,\nu}\} = \min\{\sum_{l_\nu=\pm 1} N_{l_\nu,1/2}, L^h_0\}$. This gives zero in the case of the half-filling initial ground state, in agreement with the numerical results of Ref. \cite{67}.

The number $\nu$ equals the length of the ideal charge Takahashi’s string excitations associated with the $c, \nu$ pseudoparticle branch \cite{1}. We emphasize that an infinite number of the matrix elements between the initial ground state and excited states of the Lehmann representation of the $\mathcal{N}$-rotated-electron spectral function of the operator $O_{\nu}$ vanishes exactly as a consequence of the ground-state charge selection rule associated with Eq. (40). Moreover, we find later in this section that the exact $\mathcal{N}$-rotated-electron rules correspond to the dominant holon and spinon microscopic physical processes generated by application of the corresponding $\mathcal{N}$-electron operator onto the ground state. For finite values of $U/t$ less than 1% of the $\mathcal{N}$-electron spectral weight does not correspond to the final states associated with deviation values obeying the selection rule (40). Such a small amount of spectral weight corresponds to a few extra final states with deviation values outside the ranges given in Eq. (40). However, it is found in Ref. \cite{61} that...
the absolute value of the matrix elements of the spectral functions \( \langle 14 \rangle - \langle 12 \rangle \) and \( \langle 24 \rangle - \langle 23 \rangle \) decreases rapidly as the number of holon and spinon processes needed for generation of the corresponding excited states increases. It follows that also for the \( N \)-electron operator an infinite number of possible final states give no measurable contribution to the \( N \)-electron spectral weight. This property is related to the exact ground-state selection rule \( \langle 40 \rangle \) for the states generated by the corresponding \( N \)-rotated-electron operator.

In the case of \( N \)-rotated-electron operators, the absolute maximum value of the permitted values given in Eq. \( \langle 40 \rangle \) is given by \( N \). The value \( M_{c,-1/2} = N \) is reached when the operator \( \tilde{O}_N \) can be written as the product of \( N \) creation \( N \)-electron operators. Analysis of Eq. \( \langle 40 \rangle \) reveals that the general \( N \)-rotated-electron (and \( N \)-electron) excitation \( \tilde{O}_N |G\rangle \) has quantum overlap (and \( \tilde{O}_N |G\rangle \) has significant quantum overlap) only for energy eigenstates described by charge Takahashi’s ideal string excitations of length \( \nu \leq \sum_{l_c = \pm 1} N_{-1, l_c} \). In the particular case when \( \tilde{O}_N \) can be expressed as a product of \( N \) creation \( N \)-electron operators this gives \( \nu \leq N \). The number \( N \) is thus the maximum absolute value for the length of such a charge ideal string excitation that can be generated by application onto the ground state of a general \( N \)-rotated-electron operator. In the case of the excitation generated by application onto the same state of the corresponding \( N \)-electron operator more than 99% of the spectral weight is exhausted by excited states containing string excitations of length \( \nu \leq \sum_{l_c = \pm 1} N_{-1, l_c} \), as confirmed below for one-electron operators. This also gives \( \nu \leq N \) if the \( N \)-electron operator can be written as a product of \( N \) creation electronic operators.

When the initial state is a ground state the permitted values of the \(-1/2\) spinon deviation \( \Delta M_{c,-1/2} \) generated by application of the ground state of a \( N \)-rotated-electron operator are given by Eq. \( \langle 34 \rangle \), with \( \Delta M_{c,-1/2} \) restricted to the values of Eq. \( \langle 30 \rangle \). This leads to a domain of values obeying the inequality \( \langle 34 \rangle \). However, this exact spinon selection rule does not restrict the length \( \nu \) of the spin Takahashi’s ideal string excitations which have quantum overlap with \( N \)-rotated-electron excitations \( \tilde{O}_N |G\rangle \). This is because according to the expressions given in Eq. \( \langle C25 \rangle \) of the companion paper \( \pi \), the ground state occupancy of \(-1/2\) spinons is finite and given by \( M^0_{s,-1/2} = N^0_{s,1} = N^0 \). Thus one can generate both \(-1/2\) HL spinons and \( s, \nu \) pseudoparticles belonging to branches such that \( \nu > 1 \) by decomposition processes of \( s,1 \) pseudoparticles which do not change the net number of \(-1/2\) spinons. We note that the exact spinon selection rules just limit the value of the deviations of such a net number and do not limit the processes which conserve its value.

The exact selection rule \( \langle 40 \rangle \) is equivalent to the inequality \( \langle 47 \rangle \). This latter inequality reveals that the deviation in the number of \( c \) pseudoparticle holes generated by application onto a ground state of a rotated-electron operator is limited by an exact selection rule. Based on the expressions provided in the companion paper \( \pi \), one can express the number of \( c \) pseudoparticle holes and the number of \( s,1 \) pseudoparticle holes in terms of the values of \( \eta \)-spin \( S_c \) and spin \( S_s \) as follows,

\[
N^h_c = 2S_c + 2 \sum_{\nu = 1}^{\infty} \nu N_{c,\nu} = L_c + 2 \sum_{\nu = 1}^{\infty} \nu N_{c,\nu},
\]

and

\[
N^h_{s,1} = 2S_s + 2 \sum_{\nu = 1}^{\infty} (\nu - 1) N_{s,\nu} = L_s + 2 \sum_{\nu = 1}^{\infty} (\nu - 1) N_{s,\nu},
\]

respectively. Based on the symmetries between the charge and spin sectors of the 1D Hubbard model, one would expect that the values of the deviation in the number of \( s,1 \) pseudoparticle holes generated by application onto a ground state of a rotated-electron operator should also be limited. Indeed, below we find numerical evidence that within the permitted final states which obey the selection rules \( \langle 40 \rangle \) and \( \langle 47 \rangle \), there is a sub class of states that describe over 94% of the few-rotated-electron spectral weight and whose deviation values in the number of \( s,1 \) pseudoparticle holes are such that,

\[
- \sum_{l_c, l_s = \pm 1} (l_c, l_s) N_{l_c, l_s} \leq \Delta N^h_{s,1} \leq N.
\]

Note that the exact selection rule \( \langle 40 \rangle \) limits the number of \(-1/2\) Yang holons and \( c, \nu \) pseudoparticles generated by application onto a ground state of a \( N \)-rotated-electron operator \( \tilde{O}_N \). Also the states whose deviation values obey Eq. \( \langle 50 \rangle \) have the following restrictions in the number of \(-1/2\) HL spinons and \( s, \nu \) pseudoparticles belonging to \( \nu > 1 \).
systems are as for \( L \) \( \rightarrow \infty \) rule (46). The rotated-electron spectral weight associated with the permitted states whose deviation values obey the exact selection that the deviation value restrictions of Eqs. (50) and (51) refer to processes that lead to a substantial part of the one-electron removal and addition and \( \frac{U}{t} \) the maximum value on the right-hand side of Eq. (51) is the same as the corresponding \( \Delta \) does not correspond to an exact selection rule for deviations generated by rotated-electron operators. Note that provided in the table were obtained by numerical simulations and seem to confirm that, in contrast to Eq. (46), Eq. 1D Hubbard model were described by a Heisenberg isotropic spin model. Within such a scheme the one-electron excitations were in part simulated by a procedure involving a change in the number of sites of the Heisenberg chain. This procedure has similarities with the one used in Refs. (50, 51). The deviation value restrictions of Eq. (51) do not correspond to an exact selection rule but are behind the result considered surprising in Ref. [22] that for \( U \rightarrow \infty \) the relative weights provided in the Table below. We expect that for \( L \rightarrow \infty \) the value of the relative weights for one-electron removal and addition given in the Table for smaller systems are as \( U/t \rightarrow \infty \) above 98% and 94%, respectively. The numbers provided in the Table seem to confirm that the deviation value restrictions of Eqs. (50) and (51) refer to processes that lead to a substantial part of the rotated-electron spectral weight associated with the permitted states whose deviation values obey the exact selection rule (49). The \( U/t \rightarrow \infty \) results of Ref. [22] were derived by a scheme where the spin degrees of freedom of the 1D Hubbard model were described by a Heisenberg isotropic spin model. Within such a scheme the one-electron excitations were in part simulated by a procedure involving a change in the number of sites of the Heisenberg chain.  

\[
\Delta \tilde{M}_{s,-1/2} = \Delta L_{s,-1/2} + \sum_{\nu=1}^{\infty} (\nu - 1) \Delta N_{s, \nu} = 0, 1, 2, \ldots, \sum_{l_c, l_s = \pm 1} \delta_{l_c, l_s} N_{l_c, l_s}.
\]  

(51)

Here the quantity \( \tilde{M}_{s,-1/2} \) is given by,

\[
\tilde{M}_{s,-1/2} = L_{s,-1/2} + \sum_{\nu=1}^{\infty} (\nu - 1) N_{s, \nu} = M_{s,-1/2} - \sum_{\nu=1}^{\infty} N_{s, \nu}.
\]  

(52)

Note that the value of this number vanishes for the ground state. Equations (50) and (51) contain the same information.

Let us consider the specific case of one rotated-electron removal and addition. In this case the states obeying the deviation value restrictions of Eqs. (50) and (51) are such that \( \Delta N^0_{s,1} = 1 \). Since the rotated-electron spectral weight distributions are independent of the value of \( U/t \) and as \( U/t \rightarrow \infty \) rotated electrons equal electrons, we can find the latter distributions by evaluating the electron spectral weight for \( U/t \rightarrow \infty \). By use of the method reported in Ref. [22], we find that as the number of sites \( L \) increases the one \( s,1 \) pseudoparticle hole excitations have for one-electron removal and addition and \( U/t \rightarrow \infty \) the relative weights provided in the Table below. We expect that for \( L \rightarrow \infty \) the value of the relative weights for one-electron removal and addition given in the Table for smaller systems are as \( U/t \rightarrow \infty \) above 98% and 94%, respectively. The numbers provided in the Table seem to confirm that the deviation value restrictions of Eqs. (50) and (51) refer to processes that lead to a substantial part of the rotated-electron spectral weight associated with the permitted states whose deviation values obey the exact selection rule (49). The \( U/t \rightarrow \infty \) results of Ref. [22] were derived by a scheme where the spin degrees of freedom of the 1D Hubbard model were described by a Heisenberg isotropic spin model. Within such a scheme the one-electron excitations were in part simulated by a procedure involving a change in the number of sites of the Heisenberg chain. This procedure has similarities with the one used in Refs. (50, 51). The deviation value restrictions of Eq. (51) do not correspond to an exact selection rule but are behind the result considered surprising in Ref. [22] that for \( U/t \rightarrow \infty \), more than 97% and more than 99% of the spectral weight associated with creation of an electron and annihilation of an electron, respectively, is found on the spin branch of Faddeev and Takhtajan. This branch dispersion refers to the part of the one-rotated-electron spectral weight associated with the spin degrees of freedom. It is well known from the Bethe-ansatz solution that the holes in the \( c \) and \( s \) 1 pseudoparticle bands play a key role in the energy spectrum of the charge and spin excitations of the 1D Hubbard model, respectively. Note that the ground-state selection rules (49) and deviation value restrictions (51) can be expressed in terms of the deviation values of the numbers of \( c \) and \( s \) 1 pseudoparticle holes through the inequalities (47) and (50), respectively. When \( \tilde{O}_{\mathcal{N}} \) is the one-rotated-electron creation or annihilation operator, according to the ground state exact selection rule (47) and the deviation value restrictions of Eq. (50), the maximum number of holes created in the \( c \) pseudoparticle and \( s, 1 \) pseudoparticle bands respectively is one. Thus if the initial ground state has zero spin density the single \( s, 1 \) pseudoparticle hole indeed corresponds to the well known spin branch dispersion of Faddeev and Takhtajan.

Similar results are expected to hold for excitations generated by other few rotated-electron operators. The numbers provided in the table were obtained by numerical simulations and seem to confirm that, in contrast to Eq. (49), Eq. (51) does not correspond to an exact selection rule for deviations generated by rotated-electron operators. Note that the maximum value on the right-hand side of Eq. (51) is the same as the corresponding \( \Delta M_{s,-1/2} \) maximum value of the general \(-1/2\) spinon number deviation inequality (53).

B. DOMINANT PROCESSES FOR THE FEW-ELECTRON SPECTRAL PROPERTIES

Here we confirm that the ground-state charge selection rule (49) for deviations generated by \( \mathcal{N} \)-rotated-electron operators also defines the dominant holon and spinon microscopic processes that control the spectral properties of the corresponding \( \mathcal{N} \)-electron operator. The dominant processes correspond to 99.75% - 100.00% of the whole electronic spectral weight and are associated with states whose deviation values generated by application of a \( \mathcal{N} \)-electron operator onto a ground state obey Eq. (49). Within such dominant processes, there is a sub-group of simple holon and spinon processes that correspond to about 94.00% of the electronic spectral weight. These latter processes are associated with states whose deviation values generated by application of a \( \mathcal{N} \)-electron operator onto a ground state obey both Eqs. (49) and (51). (We recall that the deviation value restrictions of Eq. (51) are not exact selection rules for rotated-electron operators.)
We start by considering the specific case of one-electron addition. We recall that according to the results of the companion paper I, the number of holons $M_c = M_{c,-1/2} + M_{c,+1/2}$ and the number of spinons $M_s = M_{s,-1/2} + M_{s,+1/2}$ are such that $M_c = [N_a - N_c]$ and $M_s = N_c$, respectively. For simplicity, let us assume that the initial ground state has zero spin density. In this case the spectral-weight distribution associated with creation of a spin-up electron has the same form as the one associated with creation of a spin-down electron. Here we consider the former case. The spin-up electron operator is related by Eq. (26) to the spin-up rotated electron. Thus in the present one-electron case the selection rule (46) and the deviation value restrictions given in Eq. (51) refer to creation of a spin-up rotated electron. From the use of expressions (46), (47), (49), and (50) of the companion paper I for the electron and rotated-electron numbers in terms of the holon, spinon, and c pseudoparticle numbers, we find that in the case of creation of a spin-up rotated electron the following transitions are permitted by the selection rule (46) and by the equivalent inequality (47):

(i) Transitions such that $-\Delta N_c = \Delta N_c^h = -1$, $\Delta M_{c,-1/2} = 0$, $\Delta M_{s,-1/2} = 0$, $\Delta M_c = -1$, and $\Delta M_s = 1$. The minimal excitation energy for such transitions is zero. Within these general transitions, the transitions that also obey the restrictions (50) and (51) are such that $\Delta N_{s,1} = 0$ and $\Delta N_{s,1}^h = 1$.

(ii) Transitions such that $-\Delta N_c = \Delta N_c^h = 1$, $\Delta M_{c,-1/2} = 1$, $\Delta M_{s,-1/2} = -1$, $\Delta M_c = 1$, and $\Delta M_s = -1$. The minimal excitation energy for such transitions is $E_u$. Within these general transitions, the transitions that also obey the restrictions (50) and (51) are such that $\Delta N_{s,1} = -1$ and $\Delta N_{s,1}^h = 1$.

In the case of creation of a spin-up rotated electron the selection rule (46) imposes that $\Delta M_{c,-1/2} = 0$, $\Delta M_s = 1$ and thus that $\Delta N_s^h \leq 1$. Note that the general transitions (i) and (ii) obey such restrictions. Within these general transitions, the transitions that also obey the restrictions (51) are such that $[\Delta M_{s,-1/2} - \Delta N_{s,1}] = 0$ and thus that $\Delta N_s^h \leq 1$.

The simplest non-permitted transitions involve creation of three holes in the c pseudoparticle band and of three holons:

(iii) Transitions such that $-\Delta N_c = \Delta N_c^h = 3$, $\Delta M_{c,-1/2} = 2$, $\Delta M_{s,-1/2} = -2$, $\Delta M_c = 3$, and $\Delta M_s = -3$. The minimal excitation energy for such transitions is $2E_u$. These transitions are not permitted by the rule (46) because $\Delta M_{c,-1/2} = 2 > 1$. Within these general transitions, the transitions that obey the restrictions (50) and (51) are such that $\Delta N_{s,1} = -2$ and $\Delta N_{s,1}^h = 1$.

Within the permitted transitions of type (ii), the simplest transitions that do not obey the restrictions (50) and (51) involve creation of three holes in the s,1 pseudoparticle band:

(iii) Transitions such that $-\Delta N_c = \Delta N_c^h = 1$, $\Delta M_{c,-1/2} = 1$, $\Delta M_{s,-1/2} = -1$, $\Delta M_c = 1$, and $\Delta M_s = -1$ and with $\Delta N_{s,1} = -2$, $\Delta N_{s,1}^h = 1$. The minimal excitation energy for such transitions is $E_u$. These transitions do not obey the restrictions (51) because $[\Delta M_{s,-1/2} - \Delta N_{s,1}] = \Delta L_{s,-1/2} = 1 > 0$.

In the case of half filling we often shift the ground-state zero-energy level to the middle of the Mott-Hubbard gap. In that case the above minimal excitation energies $0$, $E_u$, and $2E_u$ become $0$, $E_{MH}/2$, and $3E_{MH}/2$, respectively, where $E_{MH} = E_u$ at $n = 1$. Below we call three-holon states the final states associated with the transitions (iii) because they involve creation of three holons. These states also involve creation of three holes in the c pseudoparticle band. Moreover, we call three-s,1-hole states the final states behind transitions (ii'), which involve creation of three holes in the s,1 pseudoparticle band. In contrast, the final states associated with both the transitions (i) and (ii) are one-holon and one s,1-hole states.

Let us now find out what the relative weight of the states (iii) (or states (iii) and (ii')) is relative to the weight of the states (i), (ii), and (ii') (or states (i) and (ii)) when all these states are generated by application onto the ground state of the spin-up electron creation operator. To assess the importance of the three-holon final states (iii) and three-s,1-hole states (ii'), first we turn to exact diagonalization of small chains. The small-chain results are
not expected to be a good approximation for the evaluation of the thermodynamic-limit weight distribution if we consider the weight associated with each specific final state. However, here we are mostly interested in the relative spectral-weight sum rules of the permitted states (i), (ii), and (ii') versus the forbidden states (iii). Moreover, we also want to know the relative weight of the states (ii'). Fortunately, we find below that in the case of such sum rules, which involve contributions from a whole class of states, the small-chain results provide values for the relative weights which agree up to 99% with the corresponding thermodynamic-limit values.

The full electron addition and removal spectrum for six sites with six electrons (half filling) is shown in Fig. 1 for a relatively large value of $U = 12t$. As mentioned above, in the case of half filling we define the Fermi level in the middle of the Mott-Hubbard gap. The Hubbard bands at $\pm E_{MH}/2$ and $\pm 3E_{MH}/2$ are well separated, and the weights at $\approx \pm 3E_{MH}/2$ are orders of magnitude smaller than the contribution of the main Hubbard bands, centered around $\pm E_{MH}/2$. The states centered around $3E_{MH}/2$ are three-holon states of type (iii). As a result of the half-filling particle-hole symmetry, there is a corresponding structure for electron removal centered around $-3E_{MH}/2$. In the large-$U/t$ limit the latter structure is associated with creation of two real-space empty sites. For the general $U/t$ case such a structure results from creation of two rotated-electron empty sites. We recall that the $\hat{M}$ summations of the few-electron spectral functions (24)-(25) refer to such a number of rotated-electron empty sites.

In Fig. 2 we have plotted the contribution of different final states to the sum rule in the case of half filling. For that reason, we have followed adiabatically the weights (matrix elements) of different states as we reduced $U/t$ (which in the present case we did for this relatively small system), and summed the weight over the particular family of states. As we can see, the contribution of the three-holon final states (iii) to the total sum rule is largest at intermediate values of $U \approx 4t$, and it does not exceed 0.25% in the total sum rule. For large values of $U/t$ it decreases as $(t/U)^4$, while for small values as $(U/t)^4$. The three-s, 1-hole contribution from the states (iv) is also less than 0.25 %, and for small values of $U/t$ it goes as $(U/t)^2$. We find below that the relative spectral weight of the final states (iii) decreases with increasing density. For instance, at quarter filling such a weight is 2% of that of half filling and vanishes in the limit of vanishing electronic density. Thus at quarter filling and $U \approx 4t$ the final states (i), (ii), and (ii') correspond to $\approx 99.99%$ of the total spectral weight and the states (iii) to $\approx 0.005%$ of such a weight. On the other hand, we know from the values of the above table that the relative weight of the states (ii') increases with increasing values of $U/t$. As we confirm below, this is not so for the states (iii), that remain having very little spectral weight as $L \to \infty$.

![Fig. 1: Electron addition ($\omega > 0$) and removal ($\omega < 0$) spectrum for the half-filled six-site ring, with $U = 12t$. Note the logarithmic scale for the weights. Not shown are the five-holon states, whose contributions are extremely small and energies are out of the shown energy window.](image)

While we couldn’t do finite size analysis due to lack of larger system sizes for arbitrary value of $U$, for large $U/t$ we have another method to calculate the contribution of the three-holon states (iii). When $U/t$ is large, it is possible to achieve a more precise statement through the systematic $t/U$ expansion of the electron - rotated-electron unitary operator $16, 11, 12$. The electron - rotated-electron canonical transformation maps the Hamiltonian onto a rotated Hamiltonian. Such a transformation applies to all operators, as given in Eq. (16). For instance, it also relates the elementary rotated electron operators to the elementary electron operators when calculating the spectral functions. So the creation operator according to the expansions $16, 11$ and $12$ can be decomposed into:

$$c_{j, \sigma}^\dagger = \cdots + c_{j, \sigma; -E_n}^\dagger + c_{j, \sigma; 0}^\dagger + c_{j, \sigma; E_n}^\dagger + c_{j, \sigma; 2E_n}^\dagger + \cdots ,$$

(53)
where the index $M$ in $c^\dagger_{j, \sigma; ME_u}$ refers to the change of rotated-electron double occupation. Although in the present large $U/t$ limit one has that $E_u \approx U$, we use the general notation $ME_u$ for labelling each Hubbard band. The operator $c^\dagger_{j, \sigma; 0} = \tilde{c}^\dagger_{j, \sigma}(1 - \hat{n}_{j, \sigma}) + O(t/U)$ adds an electron to an unoccupied site. On the other hand, $c^\dagger_{j, \sigma; E_u} = \tilde{c}^\dagger_{j, \sigma} n_{j, \sigma} + O(t/U)$ adds an electron to a site already occupied by an electron of opposite spin, thus promoting the state to the subspace with one more doubly occupied site. In the $U/t \to \infty$ limit these operators change the number of $c$ pseudoparticles and holons accordingly to the deviation values of the above transitions (i) and (ii)-(ii'), respectively.

The operator involved in the generation of the three-holon states (iii) is $c^\dagger_{j, \sigma; 2E_u}$. Its first non-vanishing term is proportional to $(t/U)^2$ and reads,

$$c^\dagger_{j, \sigma; 2E_u} = \frac{1}{U^2} \left( \left[ [\hat{T}_{E_u}, \hat{T}_0], \tilde{c}^\dagger_{j, \sigma} \hat{n}_{j, \sigma} \right] + \frac{1}{2} \left[ \hat{T}_{E_u}, \left[ \hat{T}_{E_u}, \tilde{c}^\dagger_{j, \sigma}(1 - \hat{n}_{j, \sigma}) \right] \right] \right),$$

where the rotated kinetic energy operators $\hat{T}_0$ and $\hat{T}_{E_u}$ are given in Eqs. (20) and (21), respectively. After some algebra we find,

$$c^\dagger_{j, \sigma; 2E_u} = \frac{t^2}{U^2} \left[ \tilde{c}^\dagger_{j+1, \sigma} \tilde{c}^\dagger_{j-1, \sigma} \tilde{c}^\dagger_{j, \sigma} \hat{n}_{j-1, \sigma} (1 - \hat{n}_{j, \sigma}) \hat{n}_{j+1, \sigma} \right] - \tilde{c}^\dagger_{j+1, \sigma} \tilde{c}^\dagger_{j, \sigma} \tilde{c}^\dagger_{j-1, \sigma} (1 - \hat{n}_{j-1, \sigma}) \hat{n}_{j, \sigma} \hat{n}_{j+1, \sigma} - \tilde{c}^\dagger_{j, \sigma} \tilde{c}^\dagger_{j+1, \sigma} \tilde{c}^\dagger_{j-1, \sigma} (1 - \hat{n}_{j-1, \sigma}) \hat{n}_{j, \sigma} \hat{n}_{j+1, \sigma} - \tilde{c}^\dagger_{j-1, \sigma} \tilde{c}^\dagger_{j, \sigma} \tilde{c}^\dagger_{j+1, \sigma} (1 - \hat{n}_{j-1, \sigma}) \hat{n}_{j, \sigma} \hat{n}_{j+1, \sigma} + \tilde{c}^\dagger_{j-1, \sigma} \tilde{c}^\dagger_{j, \sigma} \tilde{c}^\dagger_{j+1, \sigma} (1 - \hat{n}_{j-1, \sigma}) \hat{n}_{j, \sigma} \hat{n}_{j+1, \sigma} - \tilde{c}^\dagger_{j-1, \sigma} \tilde{c}^\dagger_{j, \sigma} \tilde{c}^\dagger_{j+1, \sigma} (1 - \hat{n}_{j-1, \sigma}) \hat{n}_{j, \sigma} \hat{n}_{j+1, \sigma} \right].$$

The operator only acts when all the $j - 1$, $j$, and $j + 1$ sites are singly occupied. The action of $c^\dagger_{j, \sigma; 2E_u}$ on sites $j - 1, j, j + 1$, apart from the $t^2/U^2$ coefficient, gives

$$|\uparrow\downarrow\downarrow\rangle \rightarrow |dee\rangle + |ded\rangle$$
$$|\downarrow\uparrow\downarrow\rangle \rightarrow -(|ded\rangle + |edd\rangle)$$
$$|\downarrow\downarrow\uparrow\rangle \rightarrow -(|ded\rangle - |edd\rangle)$$
while on any other configuration it will give zero. Here the indexes $d$ and $e$ stand for doubly-occupied sites and empty sites, respectively, and the $\uparrow$ and $\downarrow$ symbols refer to spin-up and spin-down singly-occupied sites, respectively. We can see that the operator $c_{j, \uparrow; 2E_u}^\dagger$ removes three spins with total spin $S=1/2$ (for the $S=3/2$ combination $| \uparrow\uparrow\downarrow\rangle + | \downarrow\uparrow\uparrow\rangle \rightarrow 0$).

Next, we calculate $\int A_{2UHB}^{\uparrow}(\omega)\,d\omega$, the total weight in the band centered around $3E_u/2 \approx 3U/2$ and of energy width $12t$ (each of the $e$ and $d$ sites contributes $4t$ to the bandwidth). It is given by the expectation value $\sum_{\sigma} \langle \psi_0 | c_{j, \sigma; -2E_u} c_{j, \sigma; 2E_u} | \psi_0 \rangle$, where the $| \psi_0 \rangle$ is the spin-charge factorized wave function. First we find that,

$$
\sum_{\sigma} c_{j, \sigma; -2E_u} c_{j, \sigma; 2E_u} = \frac{t^4}{U^4} \left( \frac{3}{2} - 2S_{j-1}S_j - 2S_jS_{j+1} - 2S_{j-1}S_{j+1} \right) \hat{P}_{j-1} \hat{P}_{j} \hat{P}_{j+1},
$$

where the projector $\hat{P}_{j-1} \hat{P}_{j} \hat{P}_{j+1}$ ensures the single occupation of site $j$.

Replacing the factorized wave function, the partial sum rule reads,

$$
\int A_{2UHB}^{\uparrow}(\omega)\,d\omega = \left\langle \frac{3}{2} - 2S_0 S_1 - 2S_1 S_2 - 2S_0 S_2 \right\rangle_{\text{Heis}} \langle \hat{n}_0 \hat{n}_1 \hat{n}_2 \rangle_{\text{sf}} \frac{t^4}{U^4}.
$$

Let us denote by $f^\dagger_j$ and $f_j$ the creation and annihilation operators, respectively, of a spin-less fermion at site $j$. The expectation value to find three neighboring spinless fermions is

$$
\langle \hat{n}_0 \hat{n}_1 \hat{n}_2 \rangle_{\text{sf}} = \begin{vmatrix}
\langle f^\dagger_0 f_0 \rangle & \langle f^\dagger_0 f_1 \rangle & \langle f^\dagger_0 f_2 \rangle \\
\langle f^\dagger_1 f_0 \rangle & \langle f^\dagger_1 f_1 \rangle & \langle f^\dagger_1 f_2 \rangle \\
\langle f^\dagger_2 f_0 \rangle & \langle f^\dagger_2 f_1 \rangle & \langle f^\dagger_2 f_2 \rangle
\end{vmatrix}
= n^3 - \frac{2n\sin^2(\pi n)}{\pi^2} + \frac{\sin^2(2\pi n)}{\pi^3} - \frac{n\sin^2(2\pi n)}{4\pi^2}.
$$

with the limiting behavior,

$$
\langle \hat{n}_0 \hat{n}_1 \hat{n}_2 \rangle_{\text{sf}} = \begin{cases}
\frac{4\pi^6}{135} n^3 & \text{if } n \ll 1; \\
1 - 3(1 - n) & \text{if } 1 - n \ll 1.
\end{cases}
$$

Note that the spectral weight of these states decreases rapidly away from half filling, *i.e.* at quarter filling ($n = 1/2$) it is about 2% of that at half filling.

The expectation values in the thermodynamic limit of the Heisenberg model is \cite{69},

$$
\langle S_0 S_1 \rangle_{\text{Heis}} = \frac{1}{4} - \ln 2 \approx -0.443147
$$

$$
\langle S_0 S_2 \rangle_{\text{Heis}} = \frac{1}{4} - 4 \ln 2 + \frac{9}{4} \zeta(3) \approx 0.182039
$$

so that

$$
\left\langle \frac{3}{2} - 2S_0 S_1 - 2S_1 S_2 - 2S_0 S_2 \right\rangle_{\text{Heis}} = 12 \ln 2 - \frac{9}{2} \zeta(3) \approx 2.91.
$$

The sum rule in the second upper Hubbard band defined in Sec. III is then,

$$
\int A_{2UHB}^{\uparrow}(\omega)\,d\omega \approx 2.91 \langle \hat{n}_0 \hat{n}_1 \hat{n}_2 \rangle_{\text{sf}} \frac{t^4}{U^4}.
$$

For the six-site finite-size cluster, the expectation value in Eq. \cite{69} is $(169 + 17\sqrt{13})/78 \approx 2.95$, which is about 1% off from the thermodynamic-limit value. The asymptotic $2.95t^4/U^4$ is shown in Fig. 2 as a dashed line.
Both our numerical results for general values of $U/t$ and a small system and our analytical large $U/t$ results for the thermodynamic limit confirm that the ground-state selection rule \( \frac{11}{10} \) which limits the values of the deviations generated by distribution of rotated-electron operators defines the dominant holon and spinon microscopic processes that control the spectral-weight distribution of the corresponding electronic operators. While for $U << t$ and $U >> t$ such a selection rule is exact also for these electronic operators, we find that the relative spectral weight of the permitted above states (i), (ii), and (ii') is minimum for $U \approx 4t$. This minimum value decreases with decreasing density. For half filling it is given by $\approx 99.75\%$, whereas for quarter filling it reads $\approx 99.99\%$ and in the limit of vanishing density it becomes $\approx 100.00\%$. The extremely small amount of missing spectral weight corresponds mainly to the forbidden three-holon states (iii). Higher order five-holon/five-c-hole states lead to nearly vanishing spectral weight.

While the selection rule \( \frac{11}{10} \) is exact for rotated-electron operators, the states obeying the deviation value restrictions of Eq. \( \frac{14}{10} \) correspond to final states with a single extra hole in the pseudoparticle band. However, we find that this selection rule is exact also for these electronic operators, we find that the relative spectral weight of the permitted transitions is given by $\approx 99.75\%$, whereas for quarter filling it reads $\approx 99.99\%$ and in the limit of vanishing density it becomes $\approx 100.00\%$. The extremely small amount of missing spectral weight corresponds mainly to the forbidden three-holon states (iii). Higher order five-holon/five-c-hole states lead to nearly vanishing spectral weight. Thus over $99\%$ of the one-electron addition spectral weight corresponds to generation of one holon and one and three $s$, 1 pseudoparticle holes.

A similar analysis can be performed for other few-electron operators. The deviation restrictions of Eq. \( \frac{14}{10} \) also amount to more than $99\%$ of the spectral weight generated by application onto the ground state of $N$-electron operators such that $N > 1$. Importantly, for all few-electron operators these deviation restrictions become exact both for $U << t$ and $U >> t$ and refer to the dominant holon and spinon microscopic processes for $U \approx 4t$. The spectral weight associated with excited states whose deviation values are outside the ranges defined by Eq. \( \frac{14}{10} \) is for electronic operators in general maximum for half filling, yet it remains small for such an electronic density. As an example we consider the two-electron frequency dependent optical conductivity, which is directly related to the dynamical structure factor. A preliminary finite-energy study of such a $N = 2$ electron problem was presented for the case of the 1D Hubbard model in Ref. \( \frac{63}{53} \). The ground-state selection rule of Eq. \( \frac{14}{10} \) implies that in that case the corresponding two-rotated-electron problem the permitted $-1/2$ holon number deviations are such that $\Delta M_{c,-1/2} = 0$, 1 and thus the permitted holon number deviations are $\Delta M_{c} = 0, 2$, respectively. The finite-energy absorption considered in that paper results from transitions associated with holon number deviations such that $\Delta M_{c,-1/2} = 0$ and $\Delta M_{c} = 2$. Thus contributions from excited states with holon number deviations such that $\Delta M_{c,-1/2} = 2$ and $\Delta M_{c} = 4$ are expected to correspond to less than $1\%$ of the two-electron optical conductivity spectral weight.

As for the one-electron problem, it is expected that such an extremely small amount of spectral weight is maximum yet very small at half filling. Such a prediction is confirmed by the results of Ref. \( \frac{72}{72} \). There such a finite-energy absorption was investigated for the sine-Gordon model. The absorptions represented for coupling constant $\beta^2 = 0.9$ by a solid line and a dashed line in Fig. 1 of the same reference correspond to one-soliton/one-antisoliton and two-soliton/two-antisoliton contributions, respectively. The latter absorption is very small, being multiplied by 100 in the figure. In the limit of $\beta^2 \rightarrow 1$ the sine-Gordon model acquires a $q$-spin $SU(2)$ symmetry and describes the 1D Hubbard model at half filling and small values of $U/t$. Moreover, in this limit the solitons and antisolitons become $+1/2$ holons and $-1/2$ holons, respectively. Therefore, the results of that reference are expected to be very similar to those of the half-filling Hubbard model. As $\beta^2 \rightarrow 1$ the above one-soliton/one-antisoliton and two-soliton/two-antisoliton transitions correspond to $\Delta M_{c,-1/2} = 1$ and $\Delta M_{c} = 2$ and $\Delta M_{c,-1/2} = 2$ and $\Delta M_{c} = 4$ deviations, respectively. The transitions associated with the latter deviations are forbidden for the corresponding two-rotated-electron operator. Thus in the case of the two-electron operator the contributions from these transitions are expected to amount for less than $1\%$ of the spectral weight. Such a prediction is confirmed by the smallness of the corresponding absorption, which is represented in Fig. 1 of Ref. \( \frac{72}{72} \). Similar results hold for other two-electron operators.

We emphasize that equivalent results also hold for one-electron removal. It is generally accepted that one-electron removal corresponds to final states with a single extra hole in the $c$ pseudoparticle band. However, we find that this general expectation is only true for one-rotated-electron removal. In the case of one-electron removal less than $1\%$ of the spectral weight goes again to final states with three extra $c$ pseudoparticle holes. In the particular case of half filling such final states lead to the structure of Fig. 1 which is centered around $-3E_{MH}/2$.

V. DISCUSSION AND CONCLUDING REMARKS

In this section we summarize and discuss the results obtained in this paper. Moreover, we discuss the application of the concepts and non-perturbative many-electron tools introduced here and in the companion papers\( \frac{12}{12} \) to the accomplishment of a program for the study of few-electron spectral functions at finite values of excitation energy. Such an application program is fulfilled in Refs. \( \frac{60}{61} \).
A. SUMMARY OF THE RESULTS

The holon, spinon, and c pseudoparticle description introduced in the first paper of this series and further studied in this second and in the third papers, can be used in the evaluation of matrix elements between the ground state and excited states and in the related problem of the derivation of the line shape for finite-energy few-electron spectral functions. The results of the present paper about the dominant microscopic physical processes that amount for more than 99% of the spectral weight generated by application onto the ground state of few-electron operators is useful for the success of such a program. Our theory also describes the higher-order holon and spinon processes associated with the remaining less than 1% of electronic spectral weight. Furthermore, in this paper we used the relation of rotated electrons to the quantum objects whose occupancy configurations describe the energy eigenstates, in the generalization of the concepts of lower Hubbard band and upper Hubbard bands for all values of the on-site repulsion. While the lower Hubbard band refers to zero rotated-electron double occupation final states, the $M$th upper Hubbard band corresponds to the spectral weight associated with the excited states of rotated-electron double occupation $M$. For large values of the ratio $U/t$ this definition of lower Hubbard band and upper Hubbard bands coincides with the usual one.

According to the inequalities given in Eq. (40), the maximum number of holons and spinons generated or annihilated by application of $\mathcal{N}$-rotated-electron operators onto any eigenstate of the spin $\sigma$ electron number operator is given by $\mathcal{N}$. In the particular case of excitations whose initial state is the ground state, the ranges provided in Eq. (40) refer to an exact selection rule for the deviation values generated by application onto the ground state of such $\mathcal{N}$-rotated-electron operators. The occurrence of this selection rule is a direct result of the relation of rotated electrons to the quantum objects whose occupancy configurations describe all energy eigenstates of the model. In this paper we found that the excited states associated with these permitted deviation values correspond to over 99% of the spectral weight generated by application onto the same state of the corresponding $\mathcal{N}$-electron operators. This means that over 99% of the spectral weight generated by application onto the ground state of a $\mathcal{N}$-electron operator corresponds to application onto such a state of the first operator term of the second expression of Eq. (26). Such an operator term is nothing but the $\mathcal{N}$-rotated-electron operator associated with the $\mathcal{N}$-electron operator under consideration. This interesting result reveals that application onto the ground state of an operator of the form given in Eq. (50) leads to very little spectral weight. The value $\mathcal{N}$ also determines the absolute maximum value $\nu = \mathcal{N}$ of the quantum number $\nu$ of the $c, \nu$ pseudoparticle branches which can have finite occupancy in final states generated by $\mathcal{N}$-rotated-electron operators. The number $\nu$ is also the length of the ideal charge Takahashi’s string excitations associated with the $c, \nu$ pseudoparticle branch. Therefore, the $\mathcal{N}$-rotated-electron excitations only couple to energy eigenstates described by $c$ Takahashi’s ideal string charge excitations of length $\nu$ such that $\nu \leq \mathcal{N}$. For the corresponding $\mathcal{N}$-electron excitations, the excited states described by $c$ Takahashi’s ideal string charge excitations of length $\nu$ such that $\nu > \mathcal{N}$ amount to less than 1% of the electronic spectral weight. It follows that the dominant processes generated by application onto the ground state of a $\mathcal{N}$-electron operator originate a number of $2\nu$-holon composite $c, \nu$ pseudoparticles and $-1/2$ Yang holons and a number of $c$ pseudoparticle holes whose values are within the ranges provided in Eqs. (46) and (47), respectively. We recall that for electronic densities $n \leq 1/a$ there are no $2\nu$-holon composite $c, \nu$ pseudoparticles and no $-1/2$ Yang holons in the ground state. Higher order processes originating a number of these quantum objects outside the range defined by Eqs. (46) and (47) correspond to less than 1% of the electronic spectral weight. These processes are generated by application onto the ground state of the operator given in Eq. (40).

Moreover, although the deviation value ranges provided in Eqs. (50) and (51) are not associated with an exact selection rule for rotated-electron operators, within the dominant processes that include all values for these deviations, they refer to quite important processes for the electronic spectral weight. These equations refer to ranges for the numbers of generated or annihilated $s, 1$ pseudoparticle holes and for the numbers of generated $2\nu$-spinon composite $s, \nu$ pseudoparticles such that $\nu > 1$ and $-1/2$ HL spinons, respectively. We note that for spin densities $m < n$ there are no $2\nu$-spinon composite $s, \nu$ pseudoparticles such that $\nu > 1$ and no $-1/2$ HL spinons in the ground state. For instance, in the case of one-electron addition considered in the previous section, Eq. (40) tells us that these important processes involve generation of one $s, 1$ pseudoparticle hole. We found that these processes lead to about 94% of the electronic spectral weight, whereas excited states involving the creation of three $s, 1$ pseudoparticle holes amount for more than 5% of such a spectral weight. We thus conclude that microscopic processes involving generation of more than three $s, 1$ pseudoparticle holes lead to almost no electronic spectral weight. Although in the case of the ideal spin Takahashi’s string excitations associated with the $s, \nu$ pseudoparticle branches the ranges of Eq. (51) are not exact, they correspond to a sub-class of excited states that amount to an important part of the electronic spectral weight.

The occurrence of dominant holon and spinon microscopic processes for the electronic spectral weight and how fast the contribution of higher order processes vanishes is related to a property found in Ref. (61) that plays a central role in the evaluation of the line shape for finite-energy few-electron spectral functions. While the dominant holon and spinon microscopic processes associated with Eqs. (46) and (47) amount for more than 99% of the few-electron spectral weight, the remaining less than 1% of spectral weight is mostly associated with final states involving generation of
a few more \( c, \nu \) pseudoparticles, \(-1/2\) Yang holons, and \( c \) pseudoparticle holes relative to the maximum value of the ranges provided in these equations. Also the contribution to the electronic spectral weight from excited states involving the generation of \( s, \nu \) pseudoparticles such that \( \nu > 1, -1/2 \) HL spinons, and \( s, 1 \) pseudoparticle holes decreases rapidly as the number of these quantum objects increases. It follows that excited states involving creation of a large number of the above-mentioned quantum objects lead to vanishing spectral weight. In particular, in the present thermodynamic limit the spectral weight of excited states whose generation involves an infinite number of quantum-object elementary processes vanishes exactly. Thus only processes involving generation of a finite number of quantum objects contribute to the few-electron spectral weight. This defines the Hilbert subspace of few-electron excitations. The pseudofermion description introduced in Ref. [60] refers to such a Hilbert subspace. The method for evaluation of matrix elements between the ground state and excited states introduced in Refs. [60, 61] takes into account all possible final states generated by a final number of quantum-object processes, as discussed below.

B. THE EVALUATION OF FINITE-ENERGY FEW-ELECTRON SPECTRAL FUNCTIONS

The holon, spinon, and pseudoparticle description introduced in the companion paper [1] and further studied here and in the companion paper [2] is applied in Refs. [60, 61] to the study of the few-electron spectral functions. The studies of these references provide the few-electron spectral function line shapes for all values of excitation energy. The above description is a necessary condition for the successful fulfillment of the program for evaluation of few-electron spectral functions at finite values of the excitation energy. Such a program is fulfilled in Refs. [60, 61] by application of the new concepts and paradigms introduced in this paper and in its companion papers [1, 2] as follows:

i) - The first step of the evaluation of a few-electron spectral function of the general form (11)-(12) or (24)-(25) is the expression of the corresponding few-electron operator as the expansion in terms of rotated-electron operators given by the second expression of Ref. (26);

ii) - Next, one uses the results of the companion paper [2] and express the rotated-electron operators in terms of local pseudoparticles operators, Yang-holon operators, and HL-spinon operators. Note that after use of the relation (26), the problem of the evaluation of the matrix elements of the few-electron spectral functions (12) and (25) is equivalent to the computation of matrix elements involving the elementary creation and annihilation operators of these quantum objects;

iii) - However, rather than in terms of the interacting pseudoparticles, it is more appropriate to use in the evaluation of such matrix elements the related non-interacting operational pseudofermion description introduced in Ref. [60]. Fortunately, the few-electron spectral functions can be expressed as a convolution of the pseudofermion spectral functions corresponding to each pseudofermion branch with finite occupancy in the excited states |\( M, j \rangle\) and |\( \bar{M}, j \rangle\) of the spectral-function expressions (11)-(12) and (24)-(25), respectively;

iv) - Finally, the evaluation of the spectral function for each pseudofermion branch with finite occupancy for these excited states uses the method applied to \( U/t \rightarrow \infty \) spin-less fermion operators in Ref. [22]. The energy spectra of the above excited states appearing in the spectral-function expressions (12) and (25) is obtained by direct use of the Bethe-ansatz solution and \( \eta \)-spin and spin symmetries. The state summations of these spectral-function expressions is simplified by the fact that the absolute value of the matrix elements vanishes rapidly as the number of pseudofermion processes involved in the generation from the ground state of the corresponding excited states increases. Such a rapid vanishing is an important property for the evaluation of the finite-energy few-electron spectral functions. It is directly related to the occurrence of dominant quantum-object microscopic processes.

The use of the relation (26) in the evaluation of finite-energy few-electron spectral functions [60, 61] is a consequence of the breakthrough of the companion paper [1] concerning the following two issues: First, the clarification of the relation of rotated electrons to the Bethe-ansatz quantum numbers that label the energy eigenstates; Second, the association of these quantum numbers with objects whose occupancy configurations describe the energy eigenstates. The occurrence of dominant processes found in this paper is also important for the studies of Refs. [60, 61]. In addition to contributing to the understanding of the non-perturbative microscopic physical mechanisms that control the few-electron spectral properties, our results are related to the rapid vanishing of the matrix elements as the number of processes that generate the corresponding excited states increases, as discussed above.
C. FINAL DISCUSSION AND CONCLUDING REMARKS

The complexity of the finite-energy one-electron and two-electron physics of the non-perturbative 1D Hubbard model explains why except for $U/t \to \infty$ investigations [20, 21, 22], there have not been many previous studies about this interesting problem. In this paper we found that excited states generated from the ground state by microscopic processes leading to deviation values in the ranges defined by Eq. 1 lead to more than 99% of the few-electron spectral weight. Moreover, a careful comparison of the line shape of the one-electron spectral weight for the trivial $U/t \to 0$ limit with the one obtained in Refs. 20, 21, 22 for the limit $U/t \to \infty$, seems to indicate that most spectral weight is located in the vicinity of pseudoparticle branch lines. Such lines are generated by a set of final states where one pseudoparticle or pseudoparticle hole is created for all its available band-momentum values $q$ and all remaining pseudoparticles or pseudoparticle holes are created at their Fermi points. In addition to these elementary processes, the line shape in the vicinity of these branch lines is for electronic and spin densities within the ranges $0 < n < 1/a$ and $0 < m < n$, respectively, generated by pseudoparticle - pseudoparticle hole processes in the $c$ and $s$, 1 bands. The one-electron spectral-weight distribution obtained in Ref. 71 by numerical simulations refers to intermediate values of the ratio $U/t$ such that $U/t = 4$ and displays charge and spin branch lines, in agreement with our prediction. Furthermore, this expectation is confirmed for both one-electron and few-electron spectral functions by the exact results of Ref. 61.

Consideration of all possible branch lines constructed in this way for the dominant excited states whose deviation values obey the ranges defined by Eqs. 170 and 171 for a given few-electron operator is expected to describe the main spectral lines observed in real quasi-one-dimensional materials. This expectation is confirmed in the case of the organic conductor TTF-TCNQ by the preliminary application of our results presented in Ref. 58. The separated one-electron charge and spin spectral lines observed in TTF-TCNQ by photoemission studies agree for the whole energy band width with the theoretical branch lines constructed by the above described procedure. These preliminary results confirm the interest for the study of the unusual finite-energy spectral properties of these materials of the concepts introduced in this paper.

Elsewhere the powerful method introduced in Refs. 60, 61 is used in a more detailed description of the line shape observed in TTF-TCNQ 62. While the preliminary results of Ref. 58 provide the form of the charge and spin branch lines, the detailed dependence on the excitation energy $\omega$ of the line shape in the vicinity of these lines is presented in Ref. 62. Fortunately, this more detailed study also agrees with the line shape observed in the real experiment. Elsewhere the method constructed in Refs. 60, 61 by means of the concepts and non-perturbative many-electron theoretical tools introduced here and in the companion papers [1, 2] is applied to the study of the two-electron dynamical structure factor for all values of $U/t$ 64. Moreover, a study of the phase diagram of a system of weakly coupled Hubbard chains which combines our 1D results with a Renormalization Group scheme will be also implemented 65. The results of these studies describe many of the anomalous spectral properties observed in real low-dimensional materials. In particular, they lead to spectral lines similar to the ones observed in finite-energy/frequency experimental investigations of the one-electron spectral weight distribution or organic metals 29, 55 and two-electron dynamical structure factor of Mott-Hubbard insulators 28. Our theoretical predictions also describe and successfully explain the microscopic mechanisms behind the phase phase diagram observed in quasi-one-dimensional materials 40.

Finally, the further application of the results obtained in this paper and in its companion paper [1] to the explicit evaluation of finite-energy few-electron spectral functions requires the introduction of the concepts of local pseudoparticle and effective pseudoparticle lattice. The introduction of these concepts is the main goal of the third and last paper of this series, Ref. [2].

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