Wave-Function Factorization of the Normal-Ordered 1D Hubbard Model for Finite Values of the On-site Repulsion $U$

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In this paper we find that in the thermodynamic limit and for the the ground-state normal-ordered 1D Hubbard model the wave function of the excited energy eigenstates which span the Hilbert subspace where the finite-number-electron excitations are contained factorizes for all values of the on-site Coulombian repulsion $U$. This factorization results from the absence of residual energy interactions for the pseudofermions whose occupancy configurations describe these states. Our study includes the introduction of the pseudoparticle - pseudofermion unitary transformation and of an operator algebra for both the pseudoparticles and the pseudofermions. As the corresponding pseudoparticles, the $c\nu$ pseudofermions (and $sv$ pseudofermions) are $\eta$-spin zero $2\nu$-holon composite quantum objects (and spin zero $2\nu$-spinon composite quantum objects) where $\nu = 1, 2, ...$. The pseudofermion description is the most suitable for the study of the finite-energy spectral properties of the model.

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I. INTRODUCTION

Recently there has been a renewed experimental interest in the exotic one-electron and two-electron spectral properties of quasi-1D materials [1,2,3,4]. Some of these experimental studies observed unusual finite-energy/frequency spectral properties, which are far from being well understood. For low values of the energy, the microscopic electronic properties of these materials are usually described by systems of coupled chains. For finite values of the energy larger than the transfer integrals for electron hopping between the chains, the one-dimensional (1D) Hubbard model is expected to provide a good description of the physics of these materials [2,3,4]. This is confirmed by the recent quantitative studies of Refs. [1,2,3]. Similar unusual spectral properties observed in two-dimensional (2D) high-$T_c$ superconductors could result from effective quasi-1D charge and spin transport [2,7,8]. The 1D Hubbard model is also suitable for the description of the microscopic mechanisms behind the spectral properties of the new quantum systems described by cold fermionic atoms on an optical lattice. Indeed, following the experimental studies of strongly correlated quantum systems of ultra cold bosonic atoms held in optical lattices [4], new experiments involving cold fermionic atoms (such as $^6$Li) on a 1D optical lattice formed by interfering laser fields are in progress. Provided that the electrons are replaced by such atoms, that system can be described by the above model. However, the non-perturbative nature of the 1D Hubbard model implies that the electronic creation and annihilation operators do not provide a suitable operational description for the study of the finite-energy spectral properties. Thus, the first step for the study of these properties is the introduction of a suitable operational description. Except in the limit of infinite on-site Coulombian repulsion $U \to \infty$ [11,12,13], the introduction of such a description is an open problem of great physical interest. For low values of energy, useful information about the effects of the non-perturbative electronic correlations is provided by two-component conformal-field theory [14,15,16,17,18]. Unfortunately, that method does not apply for finite values of energy.

In view of the above-mentioned finite-energy/frequency spectral properties observed in real experiments, which are far from being well understood, efforts towards the introduction of a suitable operational description to deal with the finite-energy problem are welcome. In this paper we introduce an operational representation for the 1D Hubbard model [19,20,21,22] in terms of the pseudofermions. In contrast to the related pseudoparticles of Refs. [23,24], the pseudofermions have no residual energy interactions. We find that in the thermodynamic limit the wave function of the excited energy eigenstates which span the Hilbert subspace where the finite-number-electron excitations are contained factorizes into separated contributions corresponding to different pseudofermion branches. (A finite-number-electron excitation is generated by application onto the ground state of operators whose expression involves the product of a finite number of electronic creation and/or annihilation operators.) That factorization occurs for all values of the on-site Coulombian repulsion $U$ of the ground-state normal-ordered 1D Hubbard model. The pseudofermion operational description is closely related to the pseudoparticle representation [23,24], and is the natural starting point for studies of the finite-energy/frequency finite-number-electron spectral properties. Specifically, our starting point is a holon, spinon, and c0 pseudoparticle representation recently introduced in Ref. [24], which refers to the whole Hilbert space of the model. The relation between the original electrons and these elementary quantum objects involves the concept of rotated electron. The rotated electrons are related to the electrons by a unitary transformation first introduced in...
Ref. 26. The concepts of local pseudoparticle and effective lattice widely used in this paper are introduced in Ref. 20. As a result of the wave-function factorization, the pseudofermion description is more suitable for the study of the overlap between finite-number-electron excitations and the energy eigenstates than the pseudoparticle representation.

As further discussed in Sec. V, the pseudofermion operational description introduced in this paper and the above-mentioned associated wave-function factorization are used everywhere in the construction of a pseudofermion dynamical theory 27, 28. Preliminary applications of such a theory led to a successful description of the finite-energy spectral properties observed in low-dimensional complex materials 1, 2, 3. In spite of the absence of residual energy interactions, the pseudofermions are shown to be active scatterers and scattering centers in Ref. 29, where the corresponding pseudofermion scattering theory is introduced.

The paper is organized as follows: In Sec. II the 1D Hubbard model and the rotated electrons are introduced and useful information about the pseudoparticle representation is provided. This includes the introduction of the operator algebra for the pseudoparticles. The pseudofermion description and the relationship between pseudoparticle and pseudofermion operators are introduced and discussed in Sec. III, as well as the pseudofermion anticommuting algebra. In Sec. IV the pseudofermion energy and momentum spectra are studied and the factorization of the finite-number-electron Hilbert subspace of the ground-state normal-ordered 1D Hubbard model is introduced and discussed. Finally, in Sec. V the discussion and the concluding remarks are presented.

The pseudofermion operational description and all other issues and concepts associated with that description introduced and studied in Secs. III and IV correspond to a novel approach to the present quantum problem. On the other hand, the information about the holon, spinon, and pseudoparticle representations presented in Sec. II follows the results of Ref. 25 and is a review and/or different interpretation of known methods and concepts that are needed for the introduction of the pseudofermion description.

II. THE 1D HUBBARD MODEL, ROTATED ELECTRONS, AND THE PSEUDOPIRTPARCLE DESCRIPTION

A. THE 1D HUBBARD MODEL AND ROTATED ELECTRONS

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

$$H = \hat{H}_{SO(4)} + \sum_{\alpha = c, s} \mu_{\alpha} \hat{S}_{\alpha}^z,$$

where the Hamiltonian $\hat{H}_{SO(4)} = \hat{H}_H - (U/2) \hat{N} + (U/4) N_a$ has SO(4) symmetry and $\hat{H}_H = \hat{T} + U \hat{\hat{D}}$ is the “simple” Hubbard model. Here $\hat{T} = -t \sum_{\sigma = \uparrow, \downarrow} \sum_{j=1}^{N_a} \left[ \hat{c}_{j, \sigma}^\dagger \hat{c}_{j+1, \sigma} + h.c. \right]$ is the kinetic-energy operator and $\hat{\hat{D}} = \sum_{j=1}^{N_a} \hat{n}_{j, \uparrow} \hat{n}_{j, \downarrow}$ is the electron double-occupation operator. On the right-hand side of Eq. \ref{eq:1}, $\mu_c = 2\mu$, $\mu_s = 2\mu_0 H$, $\mu_0$ is the Bohr magneton, and the number operators, $\hat{S}_{\alpha}^z = -\frac{\eta}{2}[N_a - \hat{N}]$ and $\hat{\hat{S}}_{\alpha}^z = -\frac{\eta}{2}[\hat{N}_\uparrow - \hat{N}_\downarrow]$ are the diagonal generators of the $\eta$-spin and spin $SU(2)$ algebras \ref{eq:1} \ref{eq:2} \ref{eq:3}, respectively. The Hamiltonian $\hat{H}_{SO(4)}$ of Eq. \ref{eq:1} commutes with the six generators of the $\eta$-spin and spin $SU(2)$ algebras and has SO(4) symmetry \ref{eq:1} \ref{eq:2} \ref{eq:3}.

(The off-diagonal generators of these two $SU(2)$ algebras are given in Eqs. \ref{eq:1} \ref{eq:2} of Ref. 23, respectively.) The number of lattice sites $N_a$ is considered to be large. The above electronic number operators read $\hat{N} = \sum_{\sigma = \uparrow, \downarrow} \hat{N}_\sigma$ and $\hat{\hat{N}} = \sum_{j=1}^{N_a} \hat{n}_{j, \sigma}$, where $\hat{n}_{j, \sigma} = \hat{c}_{j, \sigma}^\dagger \hat{c}_{j, \sigma}$ counts the number of spin-projection $\sigma$ electrons at real-space lattice site $j$. Moreover, the operator $\hat{c}_{j, \sigma}^\dagger$ (and $\hat{c}_{j, \sigma}$) creates (and annihilates) a spin $\sigma$ electron at lattice site $j = 1, 2, \ldots, N_a$. The electronic lattice constant is denoted by $a$ and the lattice length by $L = N_a a$ and periodic boundary conditions and the thermodynamic limit $L \to \infty$ are assumed.

The momentum operator is given by $\hat{\hat{P}} = \sum_{\sigma = \uparrow, \downarrow} \sum_k \hat{N}_\sigma(k) k$ where the spin-projection $\sigma$ momentum distribution operator reads $\hat{N}_\sigma(k) = \frac{1}{\sqrt{L}} \sum_{j=1}^{N_a} e^{ik j a} \hat{c}_{j, \sigma}$ and the operator $\hat{c}_{k, \sigma}$ (and $\hat{c}_{k, \sigma}^\dagger$) creates (and annihilates) a spin-projection $\sigma$ electron of momentum $k$. The operators $\hat{c}_{k, \sigma}^\dagger$ and $\hat{c}_{k, \sigma}$ are related to the above operators $\hat{c}_{j, \sigma}^\dagger$ and $\hat{c}_{j, \sigma}$ by the Fourier transforms $\hat{c}_{j, \sigma}^\dagger = [1/\sqrt{L}] \sum_{j=1}^{N_a} e^{ik j a} \hat{c}_{j, \sigma}$ and $\hat{c}_{k, \sigma} = [1/\sqrt{L}] \sum_{j=1}^{N_a} e^{-ik j a} \hat{c}_{j, \sigma}$, respectively.

Throughout this paper units of Planck constant one are used and the electronic charge is denoted by $-e$. The Bethe-ansatz solvability of the 1D Hubbard model \ref{eq:1} is restricted to the Hilbert subspace spanned by the lowest-weight states (LWSs) \ref{eq:1} \ref{eq:2} or highest-weight states (HWSs) \ref{eq:1} of the $\eta$-spin and spin algebras, that is by the states whose $S_\alpha$ and $S_\alpha^z$ numbers are such that $S_\alpha = -S_\alpha^z$ or $S_\alpha = S_\alpha^z$, respectively, where $\alpha = c$ for $\eta$-spin and $\alpha = s$ for spin. In this paper the $\eta$-spin and spin LWSs description of the Bethe-ansatz solution is used. In this case,
that solution describes energy eigenstates with electronic densities \( n = N/L \) and spin densities \( m = [N_1 - N_\uparrow]/L \) in the domains \( 0 \leq na \leq 1 \) and \( 0 \leq ma \leq na \), respectively. Some of the results presented in the paper correspond to the ranges \( 0 < na < 1 \) and \( 0 < ma < na \). The description of the states corresponding to the extended domains \( 0 \leq na \leq 1 : 1 \leq na \leq 2 \) and \(-na \leq ma \leq na : -(2 - na) \leq ma \leq -(2 - na)\), respectively, is achieved by application onto the latter states of off-diagonal generators of the \( \eta \)-spin and spin \( SU(2) \) algebras.

The electron - rotated-electron unitary transformation maps the electrons onto rotated electrons such that rotated-electron double occupation, no occupation, and spin-up and spin-down single occupation are good quantum numbers for all values of \( U/t \). The lattice occupied by rotated electrons is identical to the original electronic lattice. The electrons that occur in the 1D Hubbard model are called \( \alpha \) pseudoparticles and \( \nu \) pseudoparticles such that \( \alpha = c, s \) and \( \nu = 1, 2, \ldots \). (Here we call \( c \) pseudoparticles, the \( c \) pseudoparticles of Ref. \[23\].) Thus, within our notation, the general designation of \( \alpha \nu \) pseudoparticle refers to the \( \alpha \nu = \alpha \nu \) branches such that \( \nu = 0, 1, 2, \ldots \) and \( \alpha \nu = \nu \nu \) branches such that \( \nu = 1, 2, \ldots \). It is shown in Ref. \[23\] for \( \nu > 0 \) to the \( \nu \nu \) pseudoparticles and \( \eta \nu \) pseudoparticles are \( \nu \nu \)-holon and \( \nu \nu \)-spinon composite objects, respectively. Throughout this paper we follow the notation of that reference and denote the holons and spinons according to their value of \( \eta \)-spin projection \( \pm 1/2 \) and spin projection \( \pm 1/2 \), respectively. This lattice has the same length and effective \( \nu \)-holon and \( \nu \)-spinon composite (2) algebras \[23, 32\].

The electron - rotated-electron unitary transformation maps the electrons onto rotated electrons such that rotated-electron double occupation, no occupation, and spin-up and spin-down single occupation are good quantum numbers for all values of \( U/t \). The rotated-electron double occupation operator \( \tilde{c}^\dagger_{j, \sigma} \tilde{c}_{j, \sigma} \) such that \( \tilde{c}^\dagger_{j, \sigma} = \tilde{V}(U/t) c^\dagger_{j, \sigma} \tilde{V}(U/t) \) represents the rotated electrons, where \( \tilde{V}(U/t) \) denotes the electron - rotated-electron unitary operator. Similarly, \( c^\dagger_{j, \sigma} = \tilde{V}(U/t) \tilde{c}^\dagger_{j, \sigma} \tilde{V}(U/t) \). Note that \( c^\dagger_{j, \sigma} \) and \( \tilde{c}^\dagger_{j, \sigma} \) are only identical in the \( U/t \rightarrow \infty \) limit where electron double occupation becomes a good quantum number. The unitary operators \( \tilde{V}(U/t) \) and \( \tilde{V}(U/t) \) are uniquely defined for all values of \( U/t \) by Eqs. (21)-(23) of Ref. \[23\]. The electron - rotated-electron unitary transformation was introduced in Ref. \[23\]. The rotated-electron double occupation operator \( D \) given in Eq. (20) of Ref. \[24\] commutes with the 1D Hubbard model. Thus, the rotated-electron double occupation \( D \) is a good quantum number for all values of \( U/t \).

### B. THE PSEUDOPARTICLE OPERATORS

According to the studies of Ref. \[23\], there is an infinite number of pseudoparticle branches: the \( c \) pseudoparticles and the \( \alpha \nu \) pseudoparticles such that \( \alpha = c, s \) and \( \nu = 1, 2, \ldots \). (Here we call \( c \) pseudoparticles, the \( c \) pseudoparticles of Ref. \[23\].) Thus, within our notation, the general designation of \( \alpha \nu \) pseudoparticle refers to the \( \alpha \nu = \alpha \nu \) branches such that \( \nu = 0, 1, 2, \ldots \) and \( \alpha \nu = \nu \nu \) branches such that \( \nu = 1, 2, \ldots \). It is shown in Ref. \[23\] for \( \nu > 0 \) the \( \nu \nu \) pseudoparticles and \( \nu \nu \) pseudoparticles are \( \nu \nu \)-holon and \( \nu \nu \)-spinon composite objects, respectively. Throughout this paper we follow the notation of that reference and denote the holons and spinons according to their value of \( \eta \)-spin projection \( \pm 1/2 \) and spin projection \( \pm 1/2 \), respectively. This lattice has the same length and effective \( \nu \)-holon and \( \nu \)-spinon composite \( \nu \nu \)-spinon composite \( \nu \nu \)-spinon composite objects, respectively. Another limitation was the lack of a representation for the pseudoparticle operators in terms of spatial coordinates. The concepts of local \( \alpha \nu \) pseudoparticle and effective \( \alpha \nu \) lattice are summarized below.

Generation and removal of pseudoparticles is in general associated with creation and/or annihilation of electrons. Yet there are also transitions which change the numbers of these quantum objects at constant spin-projection \( \sigma \) electron numbers. Let us introduce the bare-momentum \( \alpha \nu \) pseudoparticle creation (and annihilation) operator \( b^\dagger_{q, \alpha \nu} \) (and \( b_{q, \alpha \nu} \)) which creates (and annihilates) a \( \alpha \nu \) pseudoparticle of bare momentum \( q \). In addition, the local \( \alpha \nu \) pseudoparticle creation operator \( b^\dagger_{x_j, \alpha \nu} \) and annihilation operator \( b_{x_j, \alpha \nu} \) are also introduced. These bare-momentum and local pseudoparticle operators are related as follows,

\[
  b^\dagger_{q, \alpha \nu} = \frac{1}{\sqrt{L}} \sum_{j=1}^{N^*_{\nu \nu}} e^{i q x_j} b^\dagger_{x_j, \alpha \nu}; \quad b_{q, \alpha \nu} = \frac{1}{\sqrt{L}} \sum_{j=1}^{N^*_{\nu \nu}} e^{-i q x_j} b_{x_j, \alpha \nu}.
\]

The local \( \alpha \nu \) pseudoparticle creation (and annihilation) operator \( b^\dagger_{x_j, \alpha \nu} \) (and \( b_{x_j, \alpha \nu} \)) creates (and annihilates) a local \( \alpha \nu \) pseudoparticle at the effective \( \alpha \nu \) lattice site of spatial coordinate \( x_j = a_{\alpha \nu} \mathbf{r}_j \), where \( j = 1, 2, \ldots, N^*_{\nu \nu}, N^*_{\nu \nu} \) is the number of sites defined in Eqs. (B6)-(B8) and (B11) and of Ref. \[23\], and

\[
  a_{\alpha \nu} = a \frac{N_a}{N^*_{\alpha \nu}} = L \frac{N^*_{\alpha \nu}}{N^*_{\nu \nu}},
\]

is the effective \( \alpha \nu \) lattice constant. There is an effective \( \alpha \nu \) pseudoparticle lattice for each \( \alpha \nu \) pseudoparticle branch \[20\]. This lattice has the same length \( L = N^*_{\alpha \nu} a_{\alpha \nu} \) as the original real-space lattice. For the \( \alpha \nu \) pseudoparticle
bands such that \( \nu > 0 \), the discrete bare-momentum values \( q_j \) are distributed symmetrically relative to zero, and are such that \( |q_j| \leq q_{0\nu} \). The two bare momentum values \( q = \pm q_{0\nu} \) limit the \( \alpha\nu \) pseudoparticle Brillouin zone, where \( q_{0\nu} = [\pi/a_{\alpha\nu}][1 - 1/N^*_{\alpha\nu}] \). It follows from the expressions given in Eq. (5) of Ref. [2] for the ground-state values of the number \( N^*_{\alpha\nu} \) that for the ground state the effective \( \alpha\nu \) lattice constants \( \{ a \} \) are given by \[26\],

\[
\begin{align*}
a_{d0}^0 &= a; & a_{cv}^0 &= \frac{1}{\delta}; & a_{s1}^0 &= \frac{1}{n^\uparrow}; & a_{sv}^0 &= \frac{1}{m^\downarrow};
\end{align*}
\]  

(4)

where \( \delta = (1/a - n) \) is the doping concentration. The meaning of the divergences in the value of the constants \( a_{d0}^0 \) defined in Eq. (4) is that the corresponding effective \( \alpha\nu \) lattice has no sites, i.e. \( N^*_{\alpha\nu} = 0 \) and, therefore, does not exist for the ground state. This is the case of the effective \( cv \) lattices for half filling when \( \nu > 0 \) and of the effective \( sv \) lattices for zero spin density when \( \nu > 1 \). It follows that such singularities just indicate the collapse of the corresponding effective \( \alpha\nu \) lattice. This is one of the reasons why some of the expressions given in this paper refer to electronic densities \( 0 < na < 1 \) and spin densities \( 0 < ma < na \), such that all ground-state effective \( \alpha\nu \) lattice constants \[34\] have finite values.

As found below, the effective \( \alpha\nu \) pseudoparticle and \( \alpha\nu \) pseudofermion lattices are identical. From use of expressions \[4\] for the ground-state effective-lattice constants \( a_{d0}^0 \), one can write the ground-state number \( N^*_{\alpha\nu} \) given in Eq. (5) of Ref. \[5\] as \( N^*_{\alpha\nu} = L/a_{d0}^0 \). Except for terms of order 1/\( L \), the limiting bare-momentum values defined in Eqs. (B14), (B16), and (B17) of Ref. \[22\] simplify and are given by \( q_{0\nu} = \pi/a_{d0}^0 \). The ground-state expressions for these \( \alpha\nu \) pseudoparticle limiting bare-momentum values can be rewritten in terms of the original electronic lattice constant \( a \) as,

\[
q_{0\nu} = \frac{\pi}{a}; \quad q_{s1}^0 = k_{F\uparrow}^\downarrow; \quad q_{cv}^0 = [\pi/a - 2k_F^\downarrow], \quad \nu > 0; \quad q_{sv}^0 = [k_{F\uparrow} - k_{F\downarrow}], \quad \nu > 1.
\]  

(5)

The conjugate variable of the bare-momentum \( q_j \) of the \( \alpha\nu \) pseudoparticle branch is the above space coordinate \( x_j \) of the corresponding effective \( \alpha\nu \) lattice. This is different to the electronic operators, where the conjugate variable of the momentum \( k_j \) is the space variable of the original electronic lattice. In reference \[20\], the pseudoparticle site distribution configurations in the effective \( \alpha\nu \) lattices that describe the energy eigenstates are related to the corresponding rotated-electron site distribution configurations.

The \( \alpha\nu \) pseudoparticle bare-momentum distribution functions \( N_{\alpha\nu}(q) \) play an important role in the pseudoparticle description \[23\]. These functions are for all energy eigenstates the eigenvalues of the following pseudoparticle bare-momentum distribution operators,

\[
\hat{N}_{\alpha\nu}(q) = b_{q,\alpha\nu}^\dagger b_{q,\alpha\nu}.
\]  

(6)

The pseudoparticles obey a Pauli principle relative to the bare-momentum occupancy configurations, i.e. a discrete bare-momentum value \( q_j \) can either be unoccupied or singly occupied by a pseudoparticle. Thus, the bare-momentum distribution functions read \( N_{\alpha\nu}(q_j) = 1 \) for occupied discrete bare-momentum values \( q_j \) and \( N_{\alpha\nu}(q_j) = 0 \) for unoccupied discrete bare-momentum values \( q_j \). Each LWS is uniquely specified by the values of the set of distribution functions \{ \( N_{\alpha\nu}(q) \) \} such that \( \nu = 0, 1, 2, \ldots \) for \( \alpha = c \) and \( \nu = 1, 2, \ldots \) for \( \alpha = s \). Physical quantities such as the energy, depend on the values of these distribution functions and numbers through the rapidity momentum functional \( k(q) \) and rapidity functionals \( \Lambda_{\alpha\nu}(q) \) and \( \Lambda_{sv}(q) \). The value of these functionals is uniquely provided by solution of the functional integral equations (13)-(16) of Ref. \[24\]. In these equations \( k_{cv}(q) \) is the \( cv \) rapidity-momentum functional and the limiting bare-momentum values \( q_{c0}^0 \) and \( q_{0\nu} \) where \( \alpha = c, s \) and \( \nu = 1, 2, \ldots \) are given in Eqs. (B14), (B16), and (B17) of the same reference. For the particular case of the ground state these values are provided in Eq. (5). The above integral equations correspond to a functional representation of the thermodynamic Bethe-ansatz equations introduced by Takahashi \[20\]. The rapidity-momentum functional is real and the rapidity functionals are the real part of Takahashi’s ideal strings \[24\]. It is useful to introduce the following \( c0 \) rapidity functional \( \Lambda_{d0}(q) \equiv \sin k(q) \) where \( k(q) \) is the rapidity-momentum functional. The ground-state values of these rapidity functionals are functions of the bare-momentum \( q \). Such functions are the inverse of the functions defined in Ref. \[23\].

Besides an operator representation for the pseudoparticles, another issue of importance for the introduction of the pseudofermion description is the definition of suitable Hilbert subspaces. For instance, an electronic ensemble space is a Hilbert subspace spanned by all energy eigenstates with the same values for the electronic numbers \( N^\uparrow \) and \( N^\downarrow \). An important concept is that of CPHS ensemble space. This is a subspace spanned by all energy eigenstates with the same values for the numbers \{ \( M_{\alpha, \pm 1/2} \) \} of \( \pm 1/2 \) holons (\( \alpha = c \)) and \( \pm 1/2 \) spinons (\( \alpha = c \)) \[23\]. In general, an electronic ensemble space contains several CPHS ensemble spaces. Moreover, usually a CPHS ensemble space includes different CPHS ensemble subspaces. A CPHS ensemble subspace is spanned by all energy eigenstates with the same
values for the sets of numbers \( N_{c0}, \{ N_{\alpha \nu} \}, \) and \( \{ L_{\alpha, -1/2} \} \) such that \( \alpha = c, s \) and \( \nu = 1, 2, \ldots \). Here \( L_{\alpha, \pm 1/2} \) denotes the number of \( \pm 1/2 \) Yang holons \( [\alpha = c] \) or \( \pm 1/2 \) HL spinons \( [\alpha = s] \). (According to the notation of Ref. \[24\], CPHS stands for \( c \) pseudoparticle, holon, and spinon.)

Another tool needed for the introduction of the pseudofermion description is the ground-state normal-ordered pseudoparticle operational representation. As further discussed below, the finite-number-electron excitations are contained in a Hilbert subspace spanned by the initial ground state and excited energy eigenstates generated from it by processes involving changes in the occupancy configurations of a finite number of \( \alpha \nu \) pseudoparticles, \( -1/2 \) Yang holons, and \( -1/2 \) HL spinons, plus a small finite density of low-energy and small-momentum \( c0 \) pseudopseudon (and \( s1 \) pseudopseudon) particle-hole processes for electronic densities \( 0 < na < 1 \) (and spin densities \( 0 < ma < na \)). Throughout this paper the symbol : \( \hat{O} \) : refers to the ground-state normal-ordered expression of a general operator \( \hat{O} \).

Such values refer to excited-energy-eigenstate deviations relative to the ground-state occupancy configurations described by the bare-momentum distribution functions and numbers given in Eqs. (C1)-(C3) of Ref. \[23\]. For these excited energy eigenstates, the \( \alpha \nu \) pseudopseudon bare-momentum distribution function and the \( -1/2 \) Yang holon and \( -1/2 \) HL spinon numbers read

\[
N_{\alpha \nu}(q) = N_{\alpha \nu}^0(q) + \Delta N_{\alpha \nu}(q); \quad L_{\alpha, -1/2} = L_{\alpha, -1/2}^0 + \Delta L_{\alpha, -1/2}.
\]

From use of the ground-state distribution and number values given in Eqs. (C1)-(C3) of Ref. \[23\], the operational relations \( \hat{N}_{\nu}(q) := \hat{N}_{\nu}(q) \) for \( \nu > 0 \), \( \hat{N}_{\nu}(q) := \hat{N}_{\nu}(q) \) for \( \nu > 1 \), and \( \hat{L}_{\alpha, -1/2} := \hat{L}_{\alpha, -1/2} \) are founded. Such relations are justified by the absence of the corresponding quantum objects in the initial ground state.

The transition from the ground state to an excited energy eigenstate leads to a shift \( Q_{c0}^0/L = 0, \pm \pi/L \) in the discrete bare-momentum value \( q_j = [2\pi/L]I_{j}^{\nu} \) of Ref. \[23\]. That shift is such that,

\[
Q_{c0}^0 = 0; \quad \sum_{\alpha=c, s} \sum_{\nu=1}^{\infty} \Delta N_{\alpha \nu} \text{ even}; \quad Q_{c0}^0 = \pm \pi; \quad \sum_{\alpha=c, s} \sum_{\nu=1}^{\infty} \Delta N_{\alpha \nu} \text{ odd};
\]

\[
Q_{\alpha \nu}^0 = 0; \quad \Delta N_{c0} + \Delta N_{\alpha \nu} \text{ even}; \quad Q_{\alpha \nu}^0 = \pm \pi; \quad \Delta N_{c0} + \Delta N_{\alpha \nu} \text{ odd}; \quad \alpha = c, s, \ \nu > 0.
\]
respectively. The anticommutators involving the creation and/or annihilation operators of these two pseudoparticles read,

\[ \{ b_{q, \alpha \nu}^\dagger, b_{q', \alpha' \nu'} \} = \delta_{\alpha, \alpha'} \delta_{\nu, \nu'} \delta_{q, q'} Q_{\alpha \nu}^0/2 = 0 \]

\[ = \frac{i}{L} \frac{\delta_{\alpha, \alpha'} \delta_{\nu, \nu'}}{e^{\pi i (q - q')/2 \sin(|q - q'|/2)}}, \quad Q_{\alpha \nu}^0/2 = \pm \pi/2, \quad (12) \]

and the anticommutators between two \( \alpha \nu \) pseudoparticle creation or annihilation operators vanish.

### III. THE PSEUDOFERMION DESCRIPTION

In this section the pseudofermion operational description and the corresponding pseudoparticle - pseudofermion unitary transformation are introduced.

#### A. THE FUNCTIONAL CHARACTER OF THE CANONICAL MOMENTUM

The \( \alpha \nu \) pseudofermion has canonical momentum \( \bar{q}_j \) given by,

\[ \bar{q}_j = \bar{q}(q_j) = q_j + \frac{Q_{\alpha \nu}^0(q_j)}{L} = \frac{2\pi}{L} I_{\alpha \nu}^0 + \frac{Q_{\alpha \nu}^0(q_j)}{L}; \quad j = 1, 2, ..., N_{\alpha \nu}^*. \quad (13) \]

Here \( Q_{\alpha \nu}^0(q_j)/L \) is the canonical-momentum shift functional,

\[ \frac{Q_{\alpha \nu}^0(q_j)}{L} = \frac{2\pi}{L} \sum_{\alpha' \nu'} \sum_{j' = 1}^{N_{\alpha' \nu'}^*} \Phi_{\alpha \nu, \alpha' \nu'}(q_j, q_{j'}) \Delta N_{\alpha' \nu'}(q_{j'}), \quad (14) \]

where the sum \( \sum_{\alpha' \nu'} \) runs over all \( \alpha' \nu' \) branches with finite pseudofermion occupancy in the excited energy eigenstate. Often in this paper we use the notation \( \alpha \nu \neq c0 \), \( s1 \) branches, which refers to all \( \alpha \nu \) branches except the \( c0 \) and \( s1 \) branches. Moreover, the summations \( \sum_{\alpha' \nu'} \sum_{\alpha \nu = c0, s1} \) and \( \sum_{\alpha' \nu' \neq c0, s1} \) run over all \( \alpha \nu \) branches with finite \( \alpha \nu \) pseudofermion occupancy in the corresponding state or subspace, the \( c0 \) and \( s1 \) branches only, and all \( \alpha \nu \) branches with finite \( \alpha \nu \) pseudofermion occupancy in the corresponding state or subspace except the \( c0 \) and \( s1 \) branches, respectively.

It is shown elsewhere that the function \( \pi \Phi_{\alpha \nu, \alpha' \nu'}(q, q') \) on the right-hand side of Eq. (14) is a elementary two-pseudofermion phase shift \( 29 \). In units of \( \pi \) it is given by,

\[ \Phi_{\alpha \nu, \alpha' \nu'}(q, q') = \Phi_{\alpha \nu, \alpha' \nu'}(4\pi \frac{\Lambda^0_{\alpha \nu}(q)}{U}, \frac{4\pi \Lambda^0_{\alpha' \nu'}(q')}{U}), \quad (15) \]

where \( \Phi_{\alpha \nu, \alpha' \nu'}(r, r') \) is the corresponding rapidity two-pseudofermion phase shift expressed in terms of the variable \( r \) and the ground-state rapidity function \( \Lambda^0_{\alpha \nu}(q') \) is defined in terms of its inverse function in Ref. \( 28 \). The rapidity two-pseudofermion phase shifts are the unique solutions of the integral equations \( A1 \) - \( A12 \) of Appendix A. The general expression \( 15 \) is valid for densities \( 0 < na < 1 \) and \( 0 < ma < na \). The specific two-pseudofermion phase-shift expressions involving the \( cv \neq c0 \) branches for \( na = 1 \) (and the \( sv \neq s1 \) branches for \( ma = 0 \) are studied in Ref. \( 29 \).

The functional \( Q_{\alpha \nu}(q_j)/L \) such that,

\[ Q_{\alpha \nu}(q_j)/2 = Q_{\alpha \nu}^0/2 + Q_{\alpha \nu}^0(q_j)/2, \]

gives the shift in the discrete canonical-momentum value \( \bar{q}_j \) that arises due to the transition from the ground state to an excited energy eigenstate. In turn, \( Q_{\alpha \nu}^0(q_j)/L \), Eq. \( 14 \), gives the corresponding shift in the discrete bare-momentum value \( q_j \) that arises as a result of the same transition.

The momentum shift \( Q_{\alpha \nu}^0(q_j)/L \) of Eq. \( 14 \) is the part of \( Q_{\alpha \nu}(q_j)/L \) that refers only to the canonical momentum. It fully controls the following transformation which relates the \( \alpha \nu \) pseudofermion to the corresponding \( \alpha \nu \) pseudoparticle,

\[ q_j \rightarrow \text{REPLACED BY} \rightarrow \bar{q}_j, \quad (16) \]
where \( \bar{q}_j \) is the discrete canonical-momentum defined in Eq. (13). Note that Eq. (13) and the transformation (10) apply both to the initial ground state and excited energy eigenstates, yet for the former state \( \bar{q}_j = \bar{q}_j \) because according to Eq. (14), \( Q_{0}^{c}(q_j) = 0 \). Indeed, the pseudofermion description refers to the ground-state normal-ordered 1D Hubbard model. Thus, there is a specific \( \alpha \nu \) pseudofermion description for each initial ground state. For the latter state the discrete bare momentum \( q_j = [2\pi/L]I_{q_j}^{\nu} \) of Eq. (B1) of Ref. 23 equals the discrete canonical momentum \( \bar{q}_j = q_j + Q_{0}^{p}(q_j)/L \). This justifies the designation bare momentum for \( q_j \). Thus, for the ground state the \( \alpha \nu \) pseudoparticles are identical to the \( \alpha \nu \) pseudofermions. It follows that the ground state is invariant under the pseudoparticle - pseudofermion transformation and plays the role of the vacuum of the pseudofermion theory.

The number of \( \alpha \nu \) pseudofermions, \( N_{\alpha \nu} \), equals that of \( \alpha \nu \) pseudofermions. Moreover, we introduce the \( \alpha \nu \) canonical-momentum distribution function \( N_{\alpha \nu}(\bar{q}_j) \) such that

\[
N_{\alpha \nu}(\bar{q}_j) \equiv N_{\alpha \nu}(q_j(\bar{q}_j)),
\]

where \( N_{\alpha \nu}(q_j) \) stands for the \( \alpha \nu \) pseudoparticle bare-momentum distribution function and \( q_j = q_j(\bar{q}_j) \) is the inverse function of (13). The function \( N_{\alpha \nu}(\bar{q}_j) \) is the eigenvalue of the corresponding bare-momentum number operator (10).

A scattering theory for the pseudofermions is introduced in Ref. 24. In that reference it is found that the invariance under the electron - rotated-electron unitary transformation of the \( \alpha \nu \) pseudofermions corresponding to \( \alpha \nu \) pseudoparticles created at limiting bare momentum \( q = \pm q_{0}^{\alpha \nu} \) and belonging to \( \alpha \nu \neq 0 \), s1 branches implies that each of such \( \alpha \nu \) pseudoparticles (and \( s \nu \) pseudoparticles) separates into \( 2 \nu \) independent holons (and \( 2 \nu \) independent spinons) and a \( \alpha \nu \) (and \( s \nu \)) FP scattering center. By independent holons and spinons it is meant those which remain invariant under the electron - rotated-electron transformation. (The Yang holons and HL spinons are also independent holons and spinons, respectively.) The above designation FP stands for Fermi points. Indeed, it is found in the same reference that the \( c0 \) and s1 pseudofermion and pseudofermion hole scatterers feel the created \( \alpha \nu \) (and \( s \nu \)) FP scattering centers as being \( c0 \) (and \( c0 \) and s1) pseudofermion scattering centers at the Fermi points.

As for the pseudoparticle representation, the pseudofermion description corresponds to large values of the Hubbard chain length \( L \) and is thus compatible with Takahashi’s string hypothesis 21, 23. However, while the pseudoparticle representation corresponds to the whole Hilbert space, the pseudofermion description and the associated transformation (10) refer to a Hilbert subspace called pseudofermion subspace (PS). The PS is spanned by the initial ground state and the excited energy eigenstates generated from it by the following types of processes:

(A) - A number \( N_{\text{processes}} \) of finite-energy and finite-momentum pseudofermion processes such that \( N_{\text{processes}}/N_{a} \to 0 \) as \( N_{a} \to \infty \), involving creation or annihilation of \( c0 \) and s1 pseudofermions for all values of canonical momentum away from the Fermi points and creation of pseudofermions belonging to \( \alpha \nu \neq 0 \), s1 branches whose corresponding pseudoparticles have bare-momentum values obeying the inequality \(|q| < q_{0}^{\alpha \nu} \). This can include a number \( N_{\text{phF}}^{c0} \) and \( N_{\text{phF}}^{s1} \) of finite-energy and finite-momentum \( c0 \) and s1 pseudofermion particle-hole processes, respectively, such that \( N_{\text{phF}}^{c0}/N_{a} \to 0 \) and \( N_{\text{phF}}^{s1}/N_{a} \to 0 \) as \( N_{a} \to \infty \).

(B) A number \( N_{\text{processes}} \) of processes such that \( N_{\text{processes}}/N_{a} \to 0 \) as \( N_{a} \to \infty \), including creation of independent \(-1/2 \) holons and independent \(-1/2 \) spinons and zero-energy and finite-momentum processes which change the number of \( c0 \) and s1 pseudofermions at the corresponding Fermi points. (The latter processes transform the ground-state densely packed \( c0 \) and s1 pseudofermion canonical-momentum occupancy configuration into an excited-state densely packed canonical-momentum occupancy configuration.)

(C) - For densities \( 0 < na < 1 \) and \( 0 < na < ma \), a number \( N_{\text{phF}}^{c0,i} \) and \( N_{\text{phF}}^{s1,i} \) of low-energy and small-momentum elementary \( c0 \) and s1 pseudofermion particle-hole processes in the vicinity and around the canonical-momentum values corresponding to the bare-momentum Fermi points \( q_{0}^{c0,i} \) and \( q_{0}^{s1,i} \) of Eq. (8) where \( \zeta = \pm 1 \), respectively, relative to the excited-state densely packed \( \alpha \nu = 0 \), s1 pseudofermion canonical-momentum occupancy configurations generated by the above \( c0 \) and s1 zero-energy elementary processes (B) and such that \( N_{\text{phF}}^{c0,i}/N_{a} \) and \( N_{\text{phF}}^{s1,i}/N_{a} \) vanish or remain finite but small as \( N_{a} \to \infty \).

All PS excited energy eigenstates are generated from the initial ground state by the processes of types (A)-(C). Thus, the general PS excited energy eigenstates can be written as \(|ex\rangle = G^\dagger(C) G^\dagger(B) G^\dagger(A) (GS) \), where \(|GS\rangle \) denotes the initial ground state and \( G^\dagger(A), G^\dagger(B), \) and \( G^\dagger(C) \) generate the processes (A), (B), and (C), respectively. Such generators have simple expressions in terms of pseudofermion elementary operators 25, 28.

For simplicity, densities in the ranges \( 0 < na < 1 \) and \( 0 < ma < na \) are considered. The present analysis can be extended to other values of the densities, yet for the half-filling \( na = 1 \) or zero-magnetization \( ma = 0 \) phases the excitation subspace is more reduced. The transformation associated with Eq. (10) is defined for the PS where it is unitary, as discussed below and in Appendix B. A crucial point of the pseudofermion theory is that the finite-number-electron excitations are contained in the PS. By finite-number-electron operators, it is meant here operators...
which can be written as a product of $N$ electron creation and/or annihilation operators such that $N/Na \to 0$ as $Na \to \infty$. The self-consistency of the pseudofermion theory is confirmed by the fact that the absolute value of the spectral-weight matrix elements between the initial ground state and the PS excited energy eigenstates obtained by use of the theory is a decreasing function of the number of finite-energy pseudofermion processes generated by the above operators $G^{1}(A)$ and $G^{1}(B)$, vanishing as $Na \to \infty$. Such matrix elements are derived by the pseudofermion dynamical theory reported in Refs. 27 and 28, and are fully controlled by the functional $Q_{\alpha\nu}(q)/2$ of Eq. 10. In turn, the processes (C) can involve a small finite density of elementary $c0$ and $s1$ pseudofermion particle-hole processes. Indeed, the residual interactions of the corresponding $c0$ and $s1$ pseudoparticles vanish for the subspace spanned by the excited states generated by these processes and thus the $c0$ and $s1$ pseudofermion energy remains additive in the energy contribution of each elementary process (C) even if $N_{c0,i}/Na$ and $N_{s1,i}/Na$ remain finite but small as $Na \to \infty$.

According to Eq. 10, the processes which generate the PS excited energy eigenstates from the initial ground state lead to a collective canonical-momentum shift $Q_{\alpha\nu}(q)/L = Q_{\alpha\nu}^{0}/L + Q_{\alpha\nu}^{\Phi}(q)/L$ for all the $c0$ pseudofermions and $s1$ pseudoparticles of the initial-state Fermi sea. In contrast to the pseudoparticles, the corresponding pseudofermions have no residual energy interactions. This follows from the cancelation of the $\alpha\nu$ pseudoparticle residual energy interactions by the canonical-momentum shift functional $Q_{\alpha\nu}(q)/L$ of Eq. (14). Such a cancelation is related to the form of the rapidity functionals $\Lambda_{\alpha\nu}(q)$ and rapidity-momentum functional $k(q)$ in the PS. Introduction of the pseudoparticle bare-momentum distribution functions of general form given in Eq. 14 in the rapidity functional integral equations (13)-(16) of Ref. 28 and their expansion in the small deviations 9, permits explicit solution of these equations. This procedure leads to expressions for the rapidity functionals $\Lambda_{\alpha\nu}(q)$ and rapidity-momentum functional $k(q)$ in terms of the bare-momentum distribution function deviations introduced in Eq. 9. Solution of the above-mentioned integral equations for distributions of the general form 14 leads to first-order in the deviations to expressions for the rapidity-momentum functional and rapidity functionals of the following form,

$$k(q) = k^{0}(\bar{q}(q)); \quad \Lambda_{\alpha\nu}(q) = \Lambda^{0}_{\alpha\nu}(\bar{q}(q)); \quad \alpha = c, \nu = 0, 1, 2, \ldots; \quad \alpha = s, \nu = 1, 2, \ldots.$$  (18)

Here $\bar{q}(q)$ is the $\alpha\nu$ canonical-momentum functional given in Eq. 14 with $q_{j}$ replaced by the continuum momentum $q$ and $k^{0}(q)$ and $\Lambda^{0}_{\alpha\nu}(q)$ are the corresponding ground state functions. (These ground-state functions are fully defined in terms of the corresponding inverse functions in Ref. 28). Analytical expressions for $ma = 0$ and both $U/t \to 0$ and $U/t >> 1$ are provided in Ref. 28.

It is remarkable that in the PS the functionals $\Lambda_{\alpha\nu}(q)$ and $k(q)$ equal the corresponding ground-state functions $\Lambda^{0}_{\alpha\nu}(q)$ and $k^{0}(q)$, respectively, with the bare momentum $q$ replaced by the canonical-momentum functional $\bar{q}(q)$. This property is behind the lack of pseudofermion residual energy interactions, as further discussed in Sec. IV. The canonical-momentum shift functional (14) plays a central role in the pseudofermion description of the finite-number-electron spectral properties. Indeed, the information recorded in the pseudoparticle interactions is transferred over to that functional.

The general energy spectrum of the Hamiltonian (11) depends on the quantum object occupancy configurations through the rapidity and rapidity-momentum functionals and can be written as,

$$E = E_{SO(4)} + \sum_{\alpha = c, s} \mu_{\alpha} S_{z}^{\alpha}; \quad E_{SO(4)} = E_{H} + \frac{U}{2} \left[ M_{c} - 2M_{c,-1/2} - \frac{Na}{2} \right].$$  (19)

where the expression of the energy $E_{H}$ in terms of the rapidity-momentum functional $k(q)$ and rapidity functionals $\Lambda_{\alpha\nu}(q)$ is given in Eq. (20) of Ref. 24. As further discussed in Sec. IV, it is this functional character that is behind the pseudoparticle residual energy interactions. However, by re-expression of these functionals in terms of the canonical momentum $\bar{q}$, the energy spectrum (19) can be written for the PS in terms of pseudofermion canonical-momentum distribution functions $N_{c0}(\bar{q})$ and $N_{cv}(\bar{q})$ as,

$$E = -2t \sum_{j=1}^{N_{c}} N_{c0}(\bar{q}) \cos k^{0}(\bar{q}) + 4t \sum_{\nu=1}^{\infty} \sum_{j=1}^{N_{cv}} N_{cv}(\bar{q}) \text{Re} \left\{ \sqrt{1 - (\Lambda^{0}_{cv}(\bar{q}) + i\nu U/4t)^{2}} \right\}$$

$$+ \frac{U}{2} \left[ M_{c} - \sum_{\nu=1}^{\infty} 2\nu N_{cv} - \frac{Na}{2} \right] + \sum_{\alpha} \mu_{\alpha} S_{z}^{\alpha}.$$  (20)

The term $\sum_{\alpha} \mu_{\alpha} S_{z}^{\alpha}$ is the same as on the right-hand side of Eq. 19, and $N_{cv}$ is the number of $cv$ pseudofermions.
A crucial point of the $\alpha\nu$ pseudofermion theory is the replacement of Eq. 16 of the bare-momentum $q$ by the canonical-momentum $\tilde{q} = q + Q^\Phi_{\alpha\nu}(q)/L$. Such a procedure shows formal similarities with the usual Peierls substitution. The pseudofermion, which has no residual energy interactions, is generated from the corresponding pseudoparticle by the substitution of the bare-momentum $q$ by the canonical-momentum $\tilde{q} = q + Q^\Phi_{\alpha\nu}(q)/L$. For the PS this substitution renders the general energy spectrum defined by Eq. 19 and Eq. (20) of Ref. 24 of non-interacting form for the pseudofermions, as given in Eq. 20. Indeed, since the bare-momentum distribution function dependent rapidity functionals appearing in Eq. (20) of Ref. 24 are replaced by the corresponding ground-state values $k^0(\tilde{q})$ and $\Lambda^0_{\alpha\nu}(\tilde{q})$, that are independent of the set of excited-state pseudofermion canonical-momentum distribution functions $\{N^0_{\alpha\nu}(\tilde{q})\}$, the energy (20) is linear in these functions.

The form of the general energy spectrum (20) justifies why the shake-up effects associated with the functional (14) occur in the case of the pseudofermions in the canonical momentum instead of in the energy. The dependence of the general energy spectrum (20) on that functional occurs through the canonical momentum in the argument of the ground-state rapidity and rapidity-momentum functions. Thus, these functions play the role of non-interacting spectra, since they have the same form both for the initial ground state and PS excited energy eigenstates. The shake-up effects associated with the two-pseudofermion phase shifts are thus felt by the pseudofermions as mere changes in the canonical-momentum occupancies, through the canonical-momentum shifts generated by the ground-state - excited-energy-eigenstate transitions.

The pseudoparticle bare-momentum $q_j$ description is naturally provided by the Bethe-ansatz equations 23 within Takahashi’s string hypothesis 21. We recall that the pseudoparticle discrete bare-momentum values $q_j$ are of form given in Eq. (B1) of Ref. 23 and according to Eq. (B2) of the same reference are such that $q_{j+1} - q_j = 2\pi/L$. The single discrete bare-momentum values $q_j$ are integer multiples of $2\pi/L$ or of $\pi/L$ 22 and bare-momentum contributions of order $|1/L|^2$ such that $j > 1$ have no physical significance for the pseudoparticle description: These bare-momentum contributions must be considered as equaling zero. Importantly, the same is required for the pseudofermion canonical-momentum discrete values $\tilde{q}_j$ given in Eq. 18. These discrete values are also at least of the order of $1/L$ and contributions of order $|1/L|^2$ such that $j > 1$ must be considered as equaling zero. For instance, it is straightforward to find that the discrete canonical-momentum level separation,

$$\tilde{q}_{j+1} - \tilde{q}_j = \frac{2\pi}{L} + \frac{Q^\Phi_{\alpha\nu}(q_{j+1})}{L} - \frac{Q^\Phi_{\alpha\nu}(q_j)}{L} \approx \frac{2\pi}{L},$$

is such that the second term on the right-hand side of Eq. 21 is of order $|1/L|^2$, where $\Delta q_{\alpha\nu}(q)$ is the canonical-momentum shift functional given in Eq. 14. Thus, up to first order in $1/L$ one finds that $\tilde{q}_{j+1} - \tilde{q}_j = 2\pi/L$, as for the corresponding discrete bare-momentum level separation given in Eq. (B2) of Ref. 23. However, this does not imply that to first order in $1/L$ the pseudofermion canonical-momentum equals the bare-momentum. Indeed, note that the values of the functional $Q^\Phi_{\alpha\nu}(q_j)/L$ on the right-hand side of Eq. 18 are of order $1/L$ and play a central role in the control of the finite-number-electron spectral weight distribution by the non-perturbative many-electron shake-up effects 27. What happens is that the level separation $\tilde{q}_{j+1} - \tilde{q}_j = 2\pi/L$ is valid locally in the discrete canonical-momentum space. By that we mean the following: If in the present thermodynamic limit two canonical-momentum values $\tilde{q}_j$ and $\tilde{q}_j'$ differ by a small yet finite canonical-momentum value $\Delta \tilde{q} = \tilde{q}_j - \tilde{q}_j'$, then in general $\Delta \tilde{q} \neq \frac{2\pi}{L}[j - j']$. In contrast, for the corresponding bare-momentum values it holds that $\Delta q = \frac{2\pi}{L}[j - j']$. Therefore, for small but non-vanishing canonical-momentum separation the difference $Q^\Phi_{\alpha\nu}(q_j)/L - Q^\Phi_{\alpha\nu}(q_{j'})/L$ is not anymore of order $|1/L|^2$ and thus has physical significance.

That only discrete canonical-momentum values $\tilde{q}_j$ of zero and first order in $1/L$ are physical is an important property of the pseudofermion theory. Discrete canonical-momentum values of order $|1/L|^N$ with $N > 1$ would be generated by non-linear higher-order terms of the scattering phase-shift functional $Q^\Phi_{\alpha\nu}(q)/2$ in the pseudofermion canonical-momentum distribution-function deviations $\Delta N_{\alpha'\nu'}(q')$ on the right-hand side of Eq. (10). According to the pseudofermion scattering studies of Ref. 29, such contributions would be associated with $(N + 1)$-pseudofermion phase shifts. However, it is shown in that reference that the corresponding $(N + 1)$-pseudofermion $S$ matrix factorizes into two-pseudofermion $S$ matrices.

B. PSEUDOFERMION OPERATOR ALGEBRA

The elementary creation and annihilation operators of the $\alpha\nu$ pseudofermions can be expressed in terms of the corresponding operators of the $\alpha\nu$ pseudoparticles as follows,

$$f^\dagger_{\tilde{q}_j, \alpha\nu} = \hat{V}^\dagger_{\alpha\nu} b^\dagger_{\tilde{q}_j, \alpha\nu} \hat{V}_{\alpha\nu}; \quad f_{\tilde{q}_j, \alpha\nu} = \hat{V}_\alpha^\dagger b_{\tilde{q}_j, \alpha\nu} \hat{V}_{\alpha\nu}.$$ (22)
Here $\hat{V}_{\alpha \nu}$ is a unitary operator that we call the $\alpha \nu$ pseudoparticle - pseudofermion unitary operator. In Appendix B it is shown that for the PS the operator $\hat{V}_{\alpha \nu}$ which obeys Eq. (22) is indeed unitary and given by,

$$
\hat{V}_{\alpha \nu} = \exp \left\{ \sum_{q_j} b_{q_j, \alpha \nu} [b_{q_j, +\delta(q_j, \alpha \nu)} - b_{q_j, \alpha \nu}] \right\} \delta(q_j) = Q^\dagger_{\alpha \nu}(q_j)/L.
$$

The canonical-momentum distribution function $N_{\alpha \nu}(\bar{q}_j)$ given in Eq. (17) is the eigenvalue of the operator,

$$
N_{\alpha \nu}(\bar{q}_j) = f_{\bar{q}_j, \alpha \nu}^f f_{\bar{q}_j, \alpha \nu}.
$$

Keeping only the physical momentum contributions that correspond to terms up to first order in $1/L$, the function $q_j(\bar{q}_j)$ appearing in Eq. (17) is given by,

$$
q_j = q_j(\bar{q}_j) = \bar{q}_j - \Delta q_{\alpha \nu}(\bar{q}_j) = \bar{q}_j - \frac{2\pi}{L} \sum_{\alpha' \nu'} \sum_{j'=1}^{N_{\alpha' \nu'}^{+\alpha \nu}} \Phi^f_{\alpha \nu, \alpha' \nu'}(\bar{q}_j, \bar{q}_{j'}) \Delta N_{\alpha' \nu'}(\bar{q}_{j'}). \quad (25)
$$

(We remind that since the functional $\bar{q}_j$ vanishes for the ground state, $q_j = \bar{q}_j$ for that state.) On the right-hand side of Eq. (25), $\Phi^f_{\alpha \nu, \alpha' \nu'}(\bar{q}, \bar{q}')$ is the canonical-momentum two-pseudfermion phase shift. It is defined as,

$$
\Phi^f_{\alpha \nu, \alpha' \nu'}(\bar{q}, \bar{q}') = \Phi_{\alpha \nu, \alpha' \nu'}(q(\bar{q}), q(\bar{q}')) = \Phi_{\alpha \nu, \alpha' \nu'} \left( \frac{4t \Lambda^0_{\alpha \nu}(q(\bar{q}))}{U}, \frac{4t \Lambda^0_{\alpha' \nu'}(q(\bar{q}'))}{U} \right),
$$

where $q(\bar{q})$ is the continuum version of the function $q_j$, $\Phi_{\alpha \nu, \alpha' \nu'}(q, q')$ is given in Eq. (18), $\Phi_{\alpha \nu, \alpha' \nu'}(r, r')$ is the two-pseudofermion phase shift expressed in the variable $r$ defined by the integral equations (A1)-(A12) of Appendix A, and $\Lambda^0_{\alpha \nu}(q')$ is defined in terms of its inverse function in Ref. 28.

Often one replaces the pseudoparticle bare-momentum summations by integrals and the corresponding discrete bare-momentum values $q_j$ by a continuum bare-momentum variable $q$. Since according to Eq. (B2) of Ref. 28, the difference $q_{j+1} - q_j = 2\pi/L$ is constant for all values of $j$, the use of that continuum representation involves the replacement of $\sum_{j=1}^{N_{\alpha \nu}^{+\alpha \nu}} = \sum_{q_{\alpha \nu}^{+\alpha \nu}}$ by $\frac{L}{2\pi} \int_{-q_{\alpha \nu}^{+\alpha \nu}}^{+q_{\alpha \nu}^{+\alpha \nu}} dq$. In the PS, the rapidity functional $\Lambda_{\alpha \nu}(q)$ and rapidity-momentum functional $k(q)$ equal the corresponding ground-state rapidity function $\Lambda^0_{\alpha \nu}(q)$ and rapidity-momentum function $k^0(q)$, respectively, with the bare-momentum $q$ replaced by the canonical-momentum $\bar{q}$. It follows that in the PS the limiting values of the continuum canonical-momentum $\bar{q}$ are given by the ground-state limiting values $\pm q_{\alpha \nu}^0$ given in Eq. (5). Thus, to replace the discrete canonical-momentum values by a continuum canonical-momentum variable $\bar{q}$, one must replace the summations $\sum_{j=1}^{N_{\alpha \nu}^{+\alpha \nu}} = \sum_{q_{\alpha \nu}^{+\alpha \nu}}$ by the integrals $\frac{L}{2\pi} \int_{-q_{\alpha \nu}^{+\alpha \nu}}^{+q_{\alpha \nu}^{+\alpha \nu}} dq \frac{dq(q)}{dq}$. We then introduce the canonical-momentum distribution function,

$$
N_{\alpha \nu}(\bar{q}) = \frac{dq(q)}{dq} N_{\alpha \nu}(\bar{q}). \quad (27)
$$

Here,

$$
\frac{dq(q)}{dq} = 1 - \sum_{\alpha' \nu'} \int_{-q_{\alpha' \nu'}^{+\alpha \nu}}^{+q_{\alpha' \nu'}^{+\alpha \nu}} dq' \frac{d\Phi^f_{\alpha \nu, \alpha' \nu'}(\bar{q}, \bar{q}')}{dq'} \Delta N_{\alpha' \nu'}(\bar{q}'), \quad (28)
$$

where the function $q = q(\bar{q})$ is given in Eq. (22) with $\bar{q}_j$ replaced by $\bar{q}$. The second term on the right-hand side of this equation is of first order in the canonical-momentum distribution function deviations. For the pseudofermion description only canonical-momentum and energy contributions up to first order in these deviations are physical, as further discussed below. As a result, for canonical-momentum distribution function deviations $\Delta N_{\alpha \nu}(\bar{q})$ one can consider that,

$$
\Delta N_{\alpha \nu}(\bar{q}) = \Delta N_{\alpha \nu}(\bar{q}), \quad (29)
$$
where in contrast to the case of Eq. (24) we used \( dq(\bar{q})/d\bar{q} = 1 \).

Importantly, the \( \alpha\nu \) pseudoparticle number operator,

\[
\hat{N}_{\alpha\nu} = \sum_{j=1}^{N^*_{\alpha\nu}} \hat{b}_{\bar{q},\alpha\nu} \hat{b}_{\bar{q},\alpha\nu} = \sum_{q=-\bar{q}_{\alpha\nu}^0}^{\bar{q}_{\alpha\nu}^0} \hat{b}_{q,\alpha\nu} \hat{b}_{q,\alpha\nu} = \frac{L}{2\pi} \int_{-\bar{q}_{\alpha\nu}^0}^{\bar{q}_{\alpha\nu}^0} dq \hat{b}_{\bar{q},\alpha\nu} \hat{b}_{\bar{q},\alpha\nu},
\]

is invariant under the pseudoparticle - pseudofermion transformation. It equals the \( \alpha\nu \) pseudofermion number operator,

\[
\sum_{j=1}^{N^*_{\alpha\nu}} f_{\bar{q},\alpha\nu}^\dagger f_{\bar{q},\alpha\nu} = \sum_{q=-\bar{q}_{\alpha\nu}^0}^{\bar{q}_{\alpha\nu}^0} f_{\bar{q},\alpha\nu}^\dagger f_{\bar{q},\alpha\nu} = \frac{L}{2\pi} \int_{-\bar{q}_{\alpha\nu}^0}^{\bar{q}_{\alpha\nu}^0} dq \frac{dq(\bar{q})}{d\bar{q}} f_{\bar{q},\alpha\nu}^\dagger f_{\bar{q},\alpha\nu}.
\]

As shown in Appendix B, this symmetry implies the unitary character of the \( \alpha\nu \) pseudoparticle - pseudofermion operator (23).

Moreover, the \( \nu\nu \) pseudoparticle charge and the spin and \( \eta \)-spin values found and provided in Ref. (23) are also invariant under the above transformation. The same occurs for the \( \alpha\nu \) pseudoparticle spin and spin-projection values given in that reference. The pseudoparticle - pseudofermion transformation also leaves invariant the \( \pm \frac{1}{2} \) Yang holons and \( \pm \frac{1}{2} \) HL spinons. The \( \pm \frac{1}{2} \) holon (and \( \pm \frac{1}{2} \) spinon) composite character of the \( \nu\nu \neq c0 \) pseudoparticles (and \( \alpha\nu \) pseudoparticles) also remains invariant under that transformation. It follows that the \( \nu\nu \neq c0 \) pseudofermions (and \( \alpha\nu \) pseudoparticles) are \( \eta \)-spin zero (and spin zero) composite objects of an equal number \( \nu = 1,2, \ldots \) of \( -\frac{1}{2} \) holons and \( +\frac{1}{2} \) holons (and \( -\frac{1}{2} \) spinons and \( +\frac{1}{2} \) spinons). Thus, by combining Eqs. (24) and (30) of Ref. (23) the \( \pm \frac{1}{2} \) holon (\( \alpha = c \)) and \( \pm \frac{1}{2} \) spinon (\( \alpha = s \)) number operators \( \hat{M}_{\alpha,\pm\frac{1}{2}} \) can be written in terms of pseudofermion operators as follows,

\[
\hat{M}_{\alpha,\pm\frac{1}{2}} = \hat{L}_{\alpha,\pm\frac{1}{2}} + \sum_{\nu=1}^{\infty} \sum_{q=-\bar{q}_{\alpha\nu}^0}^{\bar{q}_{\alpha\nu}^0} \nu \hat{N}_{\alpha\nu}(\bar{q}).
\]

Here the pseudofermion canonical-momentum distribution operator \( \hat{N}_{\alpha\nu}(\bar{q}) \) is given in Eq. (24) and the operator \( \hat{L}_{\alpha,\pm\frac{1}{2}} \) is the \( \pm \frac{1}{2} \) Yang holon (\( \alpha = c \)) and \( \pm \frac{1}{2} \) HL spinon (\( \alpha = s \)) number operator provided in Eq. (39) of Ref. (23).

Thus, for the PS all results reported in Ref. (23) concerning pseudoparticle charge and spin transport are also valid for the corresponding pseudofermions. For instance, for finite values of \( U/t \) the transport of charge (and spin) is associated with the \( c0 \) pseudofermion and \( \nu\nu \) pseudofermion quantum charge fluids (and \( \alpha\nu \) pseudofermion quantum spin fluids).

We recall that the bare-momentum \( q \) is the conjugate of the spatial coordinate \( x_j = a_{\alpha\nu} j \) associated with the effective \( \alpha\nu \) lattice, where \( j = 1, 2, \ldots, N^*_{\alpha\nu} \). As for the charge (or spin) carried by the pseudoparticles and of their composite character in terms of chargeons and antichargeons (23), \( \pm \frac{1}{2} \) holons, or \( \pm \frac{1}{2} \) spinons, also the effective \( \alpha\nu \) lattice remains invariant under the \( \alpha\nu \) pseudoparticle - \( \alpha\nu \) pseudofermion unitary transformation. Indeed, the functional \( Q^\Phi_{\alpha\nu}(q)/L \) which controls the pseudoparticle - pseudofermion transformation (16) does not affect the underlying effective \( \alpha\nu \) lattice. As shown in Ref. (23), for the \( \alpha\nu = c0 \), \( s1 \) branches with finite occupancy in the initial ground state, that momentum-shift functional just imposes a twisted boundary condition.

As for the case of the pseudoparticles, it is useful to introduce the local \( \alpha\nu \) pseudofermion creation operator \( f_{\bar{x},\alpha\nu}^\dagger \) and annihilation operator \( f_{\bar{x},\alpha\nu} \). These operators are related to the operators \( f_{\bar{q},\alpha\nu}^\dagger \) and \( f_{\bar{q},\alpha\nu} \), respectively, obtained from the corresponding pseudoparticle operators through the relations given in Eq. (22), as follows,

\[
f_{\bar{q},\alpha\nu}^\dagger = \frac{1}{\sqrt{N^*_{\alpha\nu}}} \sum_{j=1}^{N^*_{\alpha\nu}} e^{-i\bar{q} x_j} f_{\bar{x},\alpha\nu}^\dagger; \quad f_{\bar{q},\alpha\nu} = \frac{1}{\sqrt{N^*_{\alpha\nu}}} \sum_{j=1}^{N^*_{\alpha\nu}} e^{i\bar{q} x_j} f_{\bar{x},\alpha\nu},
\]

where the summations refer to the sites of the effective \( \alpha\nu \) lattice. The local \( \alpha\nu \) pseudofermion creation (and annihilation) operator \( f_{\bar{x},\alpha\nu}^\dagger \) (and \( f_{\bar{x},\alpha\nu} \)) creates (and annihilates) a \( \alpha\nu \) pseudofermion at the effective \( \alpha\nu \) lattice site of spatial coordinate \( x_j = a_{\alpha\nu}^0 j \), where \( j = 1, 2, \ldots, N^*_{\alpha\nu} \) and \( a_{\alpha\nu}^0 \) is the effective \( \alpha\nu \) lattice constant given in Eq. (4). (For the PS and except for \( 1/L \) corrections we can consider that the effective \( \alpha\nu \) lattice constants are the ground-state
Thus the conjugate variable of the canonical momentum \( \bar{q} \) of the \( \alpha \nu \) pseudofermion branch is the space coordinate \( x_j \) of the corresponding effective \( \alpha \nu \) lattice. The local \( \alpha \nu \) pseudoparticles and corresponding local \( \alpha \nu \) pseudofermions have the same effective \( \alpha \nu \) lattice. It follows that the local pseudoparticle and local pseudofermion site distribution configurations which describe the ground state and the PS excited energy eigenstates are the same. (These configurations are expressed in terms of rotated-electron site distribution configurations in Ref. [27].)

While the local \( \alpha \nu \) pseudoparticles and corresponding local \( \alpha \nu \) pseudofermions live in the same effective \( \alpha \nu \) lattice, the values of the set of discrete bare-momentum values \( \{q_j\} \) and canonical-momentum values \( \{\bar{q}_j\} \) such that \( j = 1, 2, \ldots, N_{\alpha \nu}' \) are different and related by Eq. (25). There is an one-to-one relation between these two sets of discrete values, which keep the same order because there is no level crossing. This property follows from the values of the discrete bare-momentum and canonical-momentum separation given in Eq. (B2) of Ref. [23] and Eq. (21), respectively.

Finally, we consider the anticommutation relations of the pseudofermion operators. It is confirmed in Refs. [27, 28] that such relations play a major role in the evaluation of finite-number-electron matrix elements between energy eigenstates. Let us consider the general situation when the canonical momenta \( \bar{q} \) and \( \bar{q}' \) of the operators \( f_{q, \alpha \nu}^{\dagger} \) and \( f_{q', \alpha \nu} \), respectively, correspond to different CPHS ensemble subspaces. The anticommutator \( \{f_{q, \alpha \nu}^{\dagger}, f_{q', \alpha \nu'}\} \) can be expressed in terms of the local-pseudofermion anticommutators \( \{f_{x_j, \alpha \nu}^{\dagger}, f_{x_j', \alpha \nu'}\} \) associated with spatial coordinates \( x_j \) and \( x_j' \) of the effective \( \alpha \nu \) and \( \alpha \nu' \) lattices, respectively, as follows:

\[
\{f_{q, \alpha \nu}^{\dagger}, f_{q', \alpha \nu'}\} = \frac{1}{\sqrt{N_{\alpha \nu}' N_{\alpha \nu}}} \sum_{j=1}^{N_{\alpha \nu}} \sum_{j'=1}^{N_{\alpha \nu}'} e^{i(q \bar{q} - q' \bar{q}')} \{f_{x_j, \alpha \nu}^{\dagger}, f_{x_j', \alpha \nu'}\}.
\]

(34)

The momentum operator, \( \hat{P} = \sum_{\sigma = \uparrow, \downarrow} \sum_k \hat{N}_\sigma(k) k \), which is the generator for the spatial translations, commutes with the unitary electron - rotated-electron transformation. Thus, it has the same expression, \( \hat{P} = \hat{\tilde{P}} = \sum_{\sigma = \uparrow, \downarrow} \sum_k \tilde{N}_\sigma(k) k \), where \( \tilde{N}_\sigma(k) = \hat{e}_k^\dagger, \hat{\sigma} \hat{e}_k \), in terms of creation and annihilation rotated-electron operators. It follows that the electronic lattice remains invariant under such a transformation and, therefore, the rotated-electron lattice and corresponding lattice constant equal those of the original electrons. Furthermore, there is a direct relation between the latter lattice and the effective \( \alpha \nu \) lattice populated by the local \( \alpha \nu \) pseudofermions associated with the operators \( f_{x_j, \alpha \nu}^{\dagger} \) and \( f_{x_j', \alpha \nu'} \). The above invariance implies that the local-pseudofermion anticommutators \( \{f_{x_j, \alpha \nu}^{\dagger}, f_{x_j', \alpha \nu'}\} \) have simple expressions. However, under the \( j \) and \( j' \) summations of Eq. (34) the the exotic functional character of the canonical-momentum values leads to the following unusual algebra for the \( \alpha \nu \) pseudofermion operators,

\[
\{f_{q, \alpha \nu}^{\dagger}, f_{q', \alpha \nu'}\} = \delta_{\alpha \nu, \alpha \nu'} \frac{1}{N_{\alpha \nu}} e^{-i(q - q') a/2} e^{i(Q_{\alpha \nu}(q) - Q_{\alpha \nu'}(q'))/2} \frac{\sin\left(\left|Q_{\alpha \nu}(q) - Q_{\alpha \nu'}(q')\right|/2\right)}{\sin\left(|q - q'| a/2\right)},
\]

(35)

and the anticommutators between two \( \alpha \nu \) pseudofermion creation or annihilation operators vanish. Here the values \( Q_{\alpha \nu}(q)/2 \) and \( Q_{\alpha \nu'}(q')/2 \) of the canonical-momentum shift functional [10] refer to the CPHS ensemble subspaces which the canonical momenta \( \bar{q} \) and \( \bar{q}' \) correspond to, respectively. A case of particular importance is when the CPHS ensemble subspaces associated with the canonical momentum \( \bar{q}' \) is that of the initial ground state. In that case \( Q_{\alpha \nu'}(q')/2 = 0 \) for the ground-state CPHS ensemble subspace and thus the anticommutation relation \( \{f_{q, \alpha \nu}^{\dagger}, f_{q', \alpha \nu'}\} \) simplifies to,

\[
\{f_{q, \alpha \nu}^{\dagger}, f_{q', \alpha \nu'}\} = \delta_{\alpha \nu, \alpha \nu'} \frac{1}{N_{\alpha \nu}} e^{-i(q - q') a/2} e^{iQ_{\alpha \nu}(q)/2} \frac{\sin\left(Q_{\alpha \nu}(q)/2\right)}{\sin\left(|q - q'| a/2\right)}.
\]

(36)

Note that if \( \sin(Q_{\alpha \nu}(q)/2) \) would vanish the anticommutation relation \( \{f_{q, \alpha \nu}^{\dagger}, f_{q', \alpha \nu'}\} \) would be the usual one, \( \{f_{q, \alpha \nu}^{\dagger}, f_{q', \alpha \nu'}\} = \delta_{\alpha \nu, \alpha \nu'} \delta_{\bar{q}, \bar{q}'} \). In contrast, in our case that quantity has in general finite values. Indeed, under nearly all ground-state - excited-energy-eigenstate transitions there is a canonical-momentum shift which results from non-perturbative shake-up effects.

For the \( \alpha \nu \neq c0 \) (and \( s \nu \neq s1 \)) pseudofermion branches the anticommutation relations [35] and [36] refer to electronic densities \( na < 1 \) (and spin densities \( m > 0 \)) such that \( N_{\alpha \nu}'/N_a \) and \( N_{\alpha \nu}''/N_a \) are finite. Fortunately, for the scattering properties only the \( c0 \) and \( s1 \) pseudofermion anticommutation relations [36] are needed [27] and thus one can study these properties for densities such that \( 0 < na \leq 1 \) and \( 0 < ma \leq na \).
Finally, comparison of Eqs. (110) and (111) for the $\alpha \nu$ pseudoparticle and $\alpha \nu$ pseudofermion anticommutators, respectively, reveals that the absence of pseudofermion residual energy interactions implies a more complicated functional character for the $\alpha \nu$ pseudofermion anticommutator. Indeed, for the pseudofermion description the whole information contained in the pseudoparticle residual interactions is transferred over to the pseudofermion anticommutator (36), through the unitary transformation described by Eqs. (16) and (22).

IV. THE PSEUDOFERMION ENERGY AND MOMENTUM SPECTRA AND THE WAVE-FUNCTION FACTORIZATION OF THE NORMAL-ORDERED 1D HUBBARD MODEL

In this section, we find that the description of the quantum problem in terms of the pseudofermions leads in the thermodynamic limit to a wave-function factorization for the PS excited energy eigenstates where the excitations generated by application onto the ground state of finite-number-electron operators are contained. Such a factorization refers to the ground-state normal-ordered 1D Hubbard model.

A. THE PSEUDOFERMION ENERGY AND MOMENTUM SPECTRA

In the PS the energy spectrum is of the form given in Eq. (20). The processes which generate the PS excited energy eigenstates from the ground state can be associated with two virtual excitations: (1) a finite number of elementary processes (A) and (B) followed by small-momentum and low-energy $c0$ pseudofermion and $s1$ pseudofermion particle-hole processes (C); (2) a collective canonical-momentum shift $Q_{\alpha \nu}(q)/L$ for all $\alpha \nu$ pseudofermions and $\alpha \nu$ pseudofermion holes with finite pseudofermion occupancy in the excited energy eigenstate. The corresponding energy deviation spectrum is derived from the general PS energy spectrum given in Eq. (20). Such a energy deviation spectrum corresponds to the ground-state normal-ordered 1D Hubbard model and reads,

$$\Delta E = \omega_0 + \sum_{j=1}^{N_u} \Delta N_{c0}(\bar{q}_j) \epsilon_{c0}(\bar{q}_j) + \sum_{j=1}^{N_{s1}} \Delta N_{s1}(\bar{q}_j) \epsilon_{s1}(\bar{q}_j) + \sum_{\alpha \nu \neq c0, s1} \sum_{j=1}^{N_{\alpha \nu}} \Delta N_{\alpha \nu}(\bar{q}_j) \epsilon_{\alpha \nu}^0(\bar{q}_j),$$

(37)

where the energy parameter $\omega_0$ is given by,

$$\omega_0 = 2\mu \Delta M_{c, -1/2} + 2\mu_0 H [\Delta M_s, -1/2 - \Delta N_{s1}].$$

(38)

Here, $\Delta M_{\alpha, -1/2}$ are the deviations in the numbers of $-1/2$ holons ($\alpha = c$) and of $-1/2$ spinons ($\alpha = s$) and $\Delta N_{s1}$ is the deviation in the number of $s1$ pseudofermions. The energy deviation spectrum (37) is additive in the $-1/2$ holon, $-1/2$ spinons, and $\alpha \nu$ pseudofermion energies. On the right-hand side of Eq. (38), the functions $\epsilon_{c0}(\bar{q})$, $\epsilon_{s1}(\bar{q})$, and $\epsilon_{\alpha \nu}^0(\bar{q})$ are the pseudofermion energy bands defined in Eqs. (C.15)-(C.21) of Ref. [23]. The zero-energy levels relative to the initial ground-state energy of these dispersions are such that,

$$\epsilon_{c0}(\pm 2k_F) = \epsilon_{s1}(\pm k_F) = \epsilon_{\alpha \nu}^0(\pm [\pi/a - 2k_F]) = \epsilon_{\alpha \nu}^0(\pm [k_{F\uparrow} - k_{F\downarrow}]) = 0.$$

(39)

Note that the above pseudofermion energy bands equal the corresponding pseudoparticle energy bands [23, 24] provided that the bare momentum $q$ is replaced by the canonical momentum $\bar{q}$. The latter bands are plotted in Figs. 6 to 9 of Ref. [24] for $m \alpha = 0$.

In Ref. [24] it is found that for the PS both the scattering-less phase shift $Q_{\alpha \nu}^0/2$ and the scattering phase shift $Q_{\alpha \nu}^0(q_j)/2$ conserve the total energy. Thus, the virtual-excitation (2) energy spectrum vanishes and the general deviation-linear energy spectrum (37) amounts to the contributions from the excitation (1). The latter PS excitation involves changes in the occupancy configurations of a finite number of quantum objects generated by the elementary processes (A) and (B) plus the small-momentum and low-energy excitations generated by the $c0$ and $s1$ pseudofermion particle-hole elementary processes (C). The excitation (2) involves a collective canonical-momentum shift of all the ground-state $c0$ pseudofermions and $s1$ pseudofermions. In the thermodynamic limit, the value of the corresponding ground-state numbers $N_{c0} = N$ and $N_{s1} = N_{\downarrow}$ approaches infinity. Thus, the self-consistency of the pseudofermion theory implies that the energy of the excitation (2) vanishes in that limit, so that the total energy is additive in the corresponding pseudofermion energies. This requirement is fulfilled because both the pseudofermion scattering events and the scattering-less phase shift $Q_{\alpha \nu}^0/2$ conserve the total energy. In contrast, the elementary processes (C)
do not involve all $c0$ and $s1$ pseudofermions, yet the corresponding densities $N_{c0,i}/Na$ and $N_{s1,i}/Na$ can reach finite but small values as $Na \rightarrow \infty$. However, we find below that in spite of these values the corresponding energy spectrum remains linear in the pseudofermion particle-hole numbers $N_{c0,i}$ and $N_{s1,i}$.

The general PS energy spectrum defined by Eq. (20) has no pseudofermion residual-interaction energy terms for it is linear in the pseudofermion canonical-momentum distribution functions. In contrast, when expressed in terms of pseudoparticle bare-momentum distribution functions it includes residual-interaction terms. In the latter case it is defined by Eq. (19) and Eq. (20) of Ref. [24]. Such residual-interaction energy terms arise from the dependence on the pseudoparticle bare-momentum distribution functions of the rapidity functionals $k(q)$ and $\Lambda_{c}(q)$ on the right-hand side of the energy expression (20) of Ref. [24]. That dependence is defined by the integral equations (13)-(16) of Ref. [23]. It is the surprising property that in the PS the rapidity functionals $k(q)$ and $\Lambda_{c}(q)$ obey the relations given in Eq. (14), where $k_{0}(q)$ and $\Lambda_{0c}(q)$ are the corresponding ground-state values, that is behind the absence of pseudofermion residual-interaction energy terms in expression (20), as discussed in Sec. III. Indeed, reexpression of the general energy spectrum defined by Eq. (19) and Eq. (20) of Ref. [24] in terms of the canonical momentum $\tilde{q}$ leads to the replacement of the functionals $k(q)$ and $\Lambda_{c}(q)$ by their ground-state values $k_{0}(q)$ and $\Lambda_{0c}(q)$, respectively. This Peierls substitution procedure leads to the PS general energy spectrum (20), which is linear in the canonical-momentum distribution functions. The non-interacting character of that energy spectrum requires that in the PS the general energy-deviation spectrum must also be linear in the pseudofermion canonical-momentum distribution-function deviations $\Delta N_{c}(\tilde{q})$ of Eq. (20). Indeed, if the energy-deviation spectrum involved non-linear contributions in the pseudofermion canonical-momentum distribution-function deviations, these quantum objects would have residual interactions. This implies that for the pseudofermion theory the higher-order energy contributions in the pseudofermion canonical-momentum distribution-function deviations have no physical meaning. This is consistent with full information about the spectral properties being retained in the functional $Q_{\alpha\nu}(q)/L$ of Eq. (13). Therefore, in order to check the consistency of the pseudofermion theory, one should confirm that in the thermodynamic limit only the energy-deviation spectrum (37) is finite, and thus that the energy terms originated by higher-order contributions in the pseudofermion canonical-momentum distribution-function deviations vanish in that limit.

In the following we confirm that energy contributions of order equal or larger than two in the canonical-momentum distribution-function deviations vanish in the thermodynamic limit. For that we use the relation $N_{c}(\tilde{q}) = N_{c}(q_{j}\tilde{q}_{j})$ given in Eq. (14). Such a relation implies that for the PS the energy contributions originated by processes of the same order in the canonical-momentum and bare-momentum distribution-function deviations differ only by the contributions of the collective shift $Q_{\alpha\nu}(\tilde{q})/L$ of the overall canonical-momentum shift $Q_{\alpha\nu}(q)/L$ associated with the excitation (2). However, since the energy contributions of the excitation (2) vanish [24], the above two energy contributions are identical, referring to the excitation (1) only.Thus, if the energy contributions in the bare-momentum distribution-function deviations of order equal or larger than two vanish in the thermodynamic limit, the same occurs for the corresponding contributions in the canonical-momentum distribution-function deviations. Moreover, we also confirm that when the ratios $N_{c0,i}/Na$ and $N_{s1,i}/Na$ remain finite but small as $Na \rightarrow \infty$, the energy spectrum associated with the elementary processes (C) is linear in the numbers $N_{c0,i}$ and $N_{s1,i}$.

For the PS both the bare-momentum and the canonical-momentum distribution-function deviations describe the elementary processes (A)-(C) which generate the excited energy eigenstates from the ground state. The processes (A) and (B) of the above excitation (1) are in finite number. Thus, in the thermodynamic limit these processes involve a vanishing density of quantum objects. Let us consider a more extended Hilbert space spanned by excited energy eigenstates involving a small but vanishing or finite density of occupied bare-momentum values for the bare-momentum distribution function deviations generated by the elementary processes of type (A) and (B). In this case, one can derive an energy functional in terms of the bare-momentum distribution function deviations $\Delta N_{c}(q)$, $\Delta N_{c}(q)$, and $\Delta N_{c}(q)$ of Eq. (9) where $\nu = 1, 2, \ldots$. This is achieved by solution of the integral equations (13)-(16) of Ref. [23] for bare-momentum distribution functions of the general form (10). Use of the obtained rapidity functional expressions in the general energy spectrum defined by Eq. (19) and Eq. (20) of Ref. [24] leads to a general energy functional of the following form,

$$\Delta E = \sum_{i=1}^{\infty} \Delta E_{i}, \quad (40)$$

where the index $i = 1, 2, \ldots$ refers to the order in the above bare-momentum distribution function deviations. (For the pseudoparticle description, the terms of order $i$ larger than one describe the residual interactions of the pseudoparti-
cles.) The first and second-order terms on the right-hand side of Eq. (40) are of the following general form,

\[ \Delta E_1 = \omega_0 + \sum_{q=-q^0_{\alpha \nu}}^{+q^0_{\alpha \nu}} \epsilon_{c0}(q) \Delta N_{c0}(q) + \sum_{q=-q^0_{\alpha \nu}}^{+q^0_{\alpha \nu}} \epsilon_{s1}(q) \Delta N_{s1}(q) + \sum_{\alpha \nu \neq c0, s1}^{+q^0_{\alpha \nu}} \epsilon_{\alpha \nu}(q) \Delta N_{\alpha \nu}(q), \]

and

\[ \Delta E_2 = \frac{1}{L} \left\{ \sum_{\alpha \nu} \sum_{q=-q^0_{\alpha \nu}}^{+q^0_{\alpha \nu}} v_{\alpha \nu}(q) Q^0_{\alpha \nu}(q) \Delta N_{\alpha \nu}(q) + \frac{1}{4\pi} \sum_{\alpha \nu = c0, s1} \sum_{j=\pm 1} \left[ Q^0_{\alpha \nu}(jq_{F\alpha \nu}) \right]^2 \right\}, \]

respectively. Here \( \Delta N_{c0}(q), \Delta N_{c\nu}(q), \) and \( \Delta N_{s\nu}(q) \) are the bare-momentum distribution function deviations given in Eq. (9) and \( \omega_0 \) is the energy functional (83). This functional is linear in the deviations \( \Delta M_{c,-1/2} \Delta M_{s,-1/2}, \) and \( \Delta N_{s1}. \) (The s1 pseudofermion number deviation of Eq. (83) corresponds to the s1 pseudoparticle number deviation.) Note that the linearity in the \(-1/2\) Yang holon and \(-1/2\) HL spinon number deviations holds for all excited energy eigenstates independently of whether the values of these deviations are small or large. That behavior follows from the non-interacting character of these quantum objects (24). The coefficients of the \( i = 1 \) linear terms are the \( \alpha \nu \) energy bands \( \epsilon_{c0}(q), \epsilon_{s1}(q), \) and \( \epsilon_{\alpha \nu}(q) \). (These bands equal the pseudofermion energy bands with the canonical-momentum \( \vec{q} \) replaced by the bare-momentum \( q \).) Importantly, note that the coefficients of the \( i = 2 \) pseudoparticle residual-interaction energy quadratic terms (12) involve the canonical-momentum-shift functional \( Q^0_{\alpha \nu}(q)/L \) defined in Eq. (14), besides the \( \alpha \nu \) group velocities \( v_{\alpha \nu}(q) = \partial \epsilon_{\alpha \nu}(q) / \partial q \) and \( v_{\alpha \nu} = v_{\alpha \nu}(q^0_{F\alpha \nu}) \). For the pseudoparticles such a functional appears in the residual-interaction energy terms, whereas for the pseudofermions it is transferred over to the canonical momentum (13) by the unitary transformation given in Eqs. (10) and (22). By use of Eq. (14) in the first expression of Eq. (12), the \( i = 2 \) energy \( \Delta E_2 \) can be expressed in terms of suitable pseudoparticle f functions \( f_{\alpha \nu, \alpha' \nu'}(q, q') \) (17, 21). This leads to \( \alpha \nu, \alpha' \nu', q, \) and \( q' \) summations of energy terms of the form \( [1/2L] f_{\alpha \nu, \alpha' \nu'}(q, q') \Delta N_{\alpha \nu}(q) \Delta N_{\alpha' \nu'}(q') \). An important property is that the coefficients of all energy terms \( E_i \) of expression (10) of order \( i > 1 \) involve only the group velocities, the two-pseudofermion phase shifts, and/or bare-momentum derivatives of these functions. For instance, note that \( E_2 \) involves the velocities and the functional \( Q^0_{\alpha \nu}(q)/2 \) of Eq. (14). This property is related to the two-pseudofermion reducibility of the \((N+1)\) pseudofermion S matrix (24). Therefore, the two-pseudofermion phase shifts control the energy expansion (10) for all deviation orders.

First, we note that although the numbers \( N_{c0,1}^{phF} \) and \( N_{s1,1}^{phF} \) of small-momentum and low-energy elementary \( c0 \) and \( s1 \) pseudofermion particle-hole processes (C) are such that the corresponding ratios \( N_{c0,1}^{phF}/N_c \) and \( N_{s1,1}^{phF}/N_s \) can reach finite but small values as \( N \to \infty \), these processes do not contribute to the value of the functional \( Q^0_{\alpha \nu}(q)/2 \). Indeed, the "particle" contributions to that functional are exactly canceled by the corresponding "hole" contributions (25). This behavior follows from the vanishing of the \( c0 \) and \( s1 \) pseudoparticle residual interactions in the subspace spanned by the excited states generated by the elementary processes (C), as confirmed by the form of the energy \( E_2 \), Eq. (12), and of the remaining energy terms \( E_i \) of expression (10) of order \( i > 2 \), which vanish when \( Q^0_{\alpha \nu}(q)/2 = 0 \). It follows that the \( c0 \) and \( s1 \) pseudofermion particle-hole processes (C) only contribute to the leading-order energy term \( E_1 \), Eq. (11), of expression (10). Thus, the energy spectrum of the small-momentum and low-energy elementary \( c0 \) and \( s1 \) pseudofermion particle-hole excitations generated by the elementary processes (C) remains linear in the number of these processes even for a small finite density of such processes.

Second, we address the issues related to the energy spectrum associated with the elementary processes (A) and (B). The energy (11) is an expansion in the bare-momentum distribution function deviations. For excited energy eigenstates whose occupancy configurations are generated by processes similar to the elementary processes (A) and (B) but involving a small finite density of occupied bare-momentum values for the bare-momentum distribution function deviations, all energy terms of deviation order \( i = 1, 2, \ldots \) are of the same order \( [1/L]^{-1} = L \) in \( 1/L \). However, here we are interested in the PS where the finite-number-electron excitations are contained. The PS excited-state deviations associated with the occupancy configurations generated by the elementary processes (A) and (B) involve a vanishing density of pseudofermions, \(-1/2\) holons, and \(-1/2\) spinons. A property of crucial importance for the pseudofermion theory is that for the bare-momentum distribution deviations corresponding to the PS excited energy eigenstates the energy terms \( E_i \) on the right-hand side of Eq. (11) associated with the excitations generated by the elementary processes (A) and (B) are of order \( [1/L]^{-i} \). Therefore, for the pseudofermion-theory thermodynamic limit only the \( i = 1 \) energy term (11) is finite, all \( i > 1 \) energy terms vanishing as \( [1/L]^{i-1} \). But according to the above considerations, since the energy contributions in the bare-momentum distribution-function deviations of order equal or larger than two vanish in the thermodynamic limit, the same occurs for the corresponding contributions in the canonical-momentum distribution-function deviations. Therefore, the fact that for the PS occupancy configurations
generated by the elementary processes (A) and (B) all energy terms $E_i$ on the right-hand side of Eq. (30) such that $i > 1$ vanish as $|1/L|^{-1}$ implies that for the thermodynamic-limit pseudofermion theory only the $i = 1$ leading energy-deviation term is finite in that limit. This is consistent with the non-interacting character of the PS general energy spectrum of Eqs. (21) for the pseudofermions. Indeed, such a non-interacting character implies that the energy-deviation spectrum is linear in the pseudofermion canonical-momentum distribution-function deviations and given by Eq. (37), as discussed above.

On the other hand, the above $f$ functions are associated with the two-pseudoparticle residual interactions and have the same role as those of Fermi-liquid theory. Indeed, for small values of the energy and electronic densities $n$ and spin densities $m$ such that $0 < na < 1$ and $0 < na < na$, respectively, the low-energy physics is controlled by the residual two-pseudoparticle interactions described by the $i = 2$ terms of the energy functional (10). Importantly, in that limit the leading-order terms in $1/L$ of that energy spectrum are of first order in $1/L$ and are contained in both the energy terms (11) and (12). On the other hand, for the pseudofermions the energy spectrum (37) vanishes in such a limit, and the same information is stored in the pseudofermion canonical-momentum (13) through the functional $Q^F_{αν}(q)/2$ of Eq. (13), as further discussed below and in Ref. 27. [For the pseudoparticles the functional $Q^F_{αν}(q)/2$ appears instead in the residual-interaction terms (12).]

In the low-energy Hilbert subspace only the $c0$ and $s1$ pseudoparticle branches have finite occupancies. In this case, as the limit of vanishing density of pseudoparticles contributing to the bare-momentum distribution-function deviations is approached, the general energy functional (10) acquires the form of the energy spectrum of a two-component $c \equiv c0$ and $s \equiv s1$ conformal field theory. The conformal dimensions that control the asymptotic of the low-energy correlations functions are extracted from the finite-size energy corrections. These energy corrections can be obtained by the use in the pseudofermion energy terms (11) and (12) of deviations $ΔN_{c0}(q)$ and $ΔN_{s1}(q)$ descriptive of general low-energy excitations. In spite that for the pseudofermion theory the energy-deviation spectrum (37) has no residual-interaction terms and thus is linear in the canonical-momentum distribution-function deviations, it is found in Ref. 25 that the above conformal dimensions arise naturally from the pseudofermion momentum for low-energy excitations.

For the pseudofermion theory, the energy (35) on the right-hand side of Eq. (37) controls the finite-energy physics. The remaining energy terms refer to gapless contributions, provided that the involved pseudofermions correspond to the canonical-momentum values in the vicinity of the energy-band arguments of Eq. (39). For most excited energy eigenstates, the latter terms also lead to finite-energy contributions. The typical value of the latter energy contributions is of the order of the pseudofermion energy dispersion band-width per pseudofermion involved in the excited energy eigenstates. Note that the PS energy spectrum (37) can have any finite value associated with the regions of the $(k, ω)$-plane where the finite-number-electron spectral functions have finite spectral weight (27).

Provided that one considers only the contributions of first-order in the canonical-momentum distribution function deviations, the momentum deviation spectrum can be written in terms of the pseudofermion canonical-momentum distribution function deviations. It is given by,

$$\Delta P = \frac{π}{a} ΔM_{cα} - 1/2 + \sum_{j=1}^{N_c} ΔN_{cα}(q) \hat{q}_j + \sum_{ν=1}^{∞} \sum_{j=1}^{N_{sν}} ΔN_{sν}(q) \hat{q}_j + \sum_{ν=1}^{∞} \sum_{j=1}^{N_{cν}} ΔN_{cν}(q) \left[ \frac{π}{a} - \hat{q}_j \right].$$

When acting onto the PS, the ground-state normal-ordered 1D Hubbard model and momentum operator can be written in terms of pseudofermion, $-1/2$ Yang holon, and $-1/2$ HL spinon operators as follows,

$$\hat{H} := \sum_{αν} \sum_{j=1}^{N_{αν}} ε_{αν}(q) \hat{q}_j \hat{q}_j^\dagger : f^{\dagger}_{q_j, αν} : f_{q_j, αν} : + \sum_{α = c,s} ε_{Lα} - 1/2 \hat{L}_α - 1/2,$$

and

$$\hat{P} := \sum_{j=1}^{N_c} \hat{q}_j \hat{q}_j^\dagger : f^{\dagger}_{q_j, c0} : f_{q_j, c0} : + \sum_{ν=1}^{∞} \sum_{j=1}^{N_{sν}} \hat{q}_j \hat{q}_j^\dagger : f^{\dagger}_{q_j, sν} : f_{q_j, sν} :$$

$$+ \sum_{ν=1}^{∞} \sum_{j=1}^{N_{cν}} [(1 + ν) \frac{π}{a} - \hat{q}_j] \hat{q}_j^\dagger : f^{\dagger}_{q_j, cν} : f_{q_j, cν} : + \frac{π}{a} \hat{L}_c - 1/2,$$

respectively, where $N^*_{c0} = N_c$ and the operator $\hat{L}_α - 1/2$ is given in Eq. (39) of Ref. 22. On the right-hand side of Eq. (44), the pseudofermion energy bands are defined by Eqs. (C.15)-(C.21) of Ref. 23 and the $-1/2$ Yang holon and $-1/2$ HL spinon energies read $24$ $ε_{Lc} - 1/2 = 2μ$ and $ε_{Ls} - 1/2 = 2μν \hat{H}$, respectively.
The ground-state normal-ordered Hamiltonian and momentum operator correspond to the energy and momentum deviation spectra given in Eqs. (37) and (43), respectively.

B. WAVE-FUNCTION FACTORIZATION OF THE NORMAL-ORDERED 1D HUBBARD MODEL

It is well known that both the ground state wave function and the wave function of the excited energy eigenstates of the 1D Hubbard model can in the $U/t \to \infty$ limit be constructed as a product of a spin-less fermion wave function and a squeezed spin wave function. In our pseudofermion language this factorization means that in such a limit the expression of the momentum and energy spectra of these states is linear in the canonical-momentum distribution functions. It is straightforward to show that for finite values of $U/t$ the general energy spectrum defined by Eq. (14) and Eq. (20) of Ref. [24] is not linear in such functions. Therefore, the above type of factorization does not occur in general for the 1D Hubbard model.

Fortunately, the evaluation of finite-number-electron spectral functions can be achieved without the full factorization of the wave functions. That problem can be solved by use of the ground-state normal-ordered 1D Hubbard model. When expressed in terms of pseudofermion operators, that Hamiltonian and associated momentum operator are given in Eqs. (44) and (45), respectively. In the thermodynamic limit, there is a wave-function factorization for the PS excited energy eigenstates. This factorization follows from the linear dependence on the canonical-momentum distribution-function deviations of the expressions (47) and (50) for the energy and momentum, respectively. Therefore, the wave function of the energy eigenstates of the normal-ordered Hamiltonian can be expressed in the PS as a product of wave functions. Each wave function corresponds to a different pseudofermion branch. In excited energy eigenstates with finite independent $-1/2$ holon and independent $-1/2$ spinon occupancy, there is also a wave function for these objects. In contrast, for the pseudoparticle representation the energy functional includes bare-momentum distribution function deviation non-linear terms associated with the pseudoparticle residual interactions. For the pseudoparticle representation we cannot ignore such energy terms because they control the low-energy physics. The occurrence of these energy terms mixes contributions from different branches. It follows that the pseudoparticle energy spectrum is not additive in the $\alpha\nu$ pseudoparticle branch contributions, in contrast to the pseudofermion energy spectrum given in Eqs. (37). Thus, in this case the wave function of the excited energy eigenstates does not factorize in the form of a product of pseudoparticle wave functions.

The number of wave functions contributing to the factorized wave function of a given energy eigenstate depends on the occupancy configurations of that state. Only the $\alpha\nu$ pseudofermion branches with finite occupancy in the state contribute to the wave function. This contribution is in the form of an $\alpha\nu$ wave function factor, as further discussed in Refs. [27, 28]. The same applies to the occupancy of independent $-1/2$ holons and independent $-1/2$ spinons.

V. CONCLUDING REMARKS

In this paper we introduced a pseudofermion operational description for the ground-state normal-ordered 1D Hubbard model. We found that in the thermodynamic limit the wave function of excited energy eigenstates belonging to the PS where the finite-number-electron excitations are contained factorizes for all values of $U/t$. This factorization results from the absence of residual-interaction energy terms for the pseudofermions whose occupancy configurations describe these excited energy eigenstates. Our study included the introduction of the pseudoparticle - pseudofermion unitary transformation and of an operator algebra for both the pseudoparticles and pseudofermions. In the PS the functional $Q_{\alpha\nu}^c(q)/L$ associated with that transformation exactly cancels the residual interactions of the $\alpha\nu$ pseudoparticles, through a mechanism similar to the usual Peierls substitution. The information recorded in the pseudoparticle interactions is contained in that functional and is transferred over to the pseudofermion canonical momentum. Moreover, we introduced creation and annihilation operators for both the pseudoparticles and pseudofermions and derived the anticommutation relations of these operators. The pseudofermion anticommutation relations play a central role in the study of the spectral and dynamical properties.

The pseudofermion operator algebra introduced here is used in Refs. [27, 28] in the construction of a pseudofermion dynamical theory. That theory allows the evaluation of finite-number-electron spectral-function expressions for all energy values. Furthermore, the pseudofermion operational description is useful for the further understanding of the exotic properties displayed by low-dimensional materials. A preliminary application of the pseudofermion dynamical theory to the study of the one-electron spectral functions is presented in Refs. [1, 3]. The theoretical predictions of these references describe quantitatively for the whole finite-energy band width the one-electron removal spectral lines observed by photoemission experiments in the quasi-1D organic compound TTF-TCNQ. Also the predictions of Ref. [6] are consistent with the phase diagram observed in a series of organic compounds. Recently, the one-electron problem investigated in Refs. [1, 3] was studied by the dynamical density matrix renormalization group.
method in Ref. [34]. The studies of the latter reference reached results similar to those of the former references. The pseudofermion description introduced here is also of interest for the understanding of the spectral properties of the new quantum systems described by cold fermionic atoms on an optical lattice.

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APPENDIX A: THE RAPIDITY TWO-PSEUDOFERMION PHASE SHIFTS $\Phi_{\alpha\nu, \alpha'\nu'}(r, r')$

Here we provide the set of integral equations which define the rapidity two-pseudofermion phase shifts $\Phi_{\alpha\nu, \alpha'\nu'}(r, r')$ in units of $\pi$ on the right-hand side of Eqs. [15]. Let us start by introducing the following Fermi surface parameters $r_0^c = 4t \sin Q/U$ and $r_0^v = 4t B/U$ where the parameters $Q$ and $B$ are defined in Ref. [28]. In order to derive the integral equations which define the rapidity two-pseudofermion phase shifts $\Phi_{\alpha\nu, \alpha'\nu'}(r, r')$, we first use in Eqs. (13)-(16) of Ref. [22] the bare-momentum distribution functions of the general form [10]. Expansion of the obtained equations up to first order in the bare-momentum distribution function deviations on the right-hand side of Eqs. [9] and [16] leads to expression [15] with the two-pseudofermion phase shift $\Phi_{\alpha\nu, \alpha'\nu'}(r, r')$ uniquely defined by the integral equations given below. A first group of two-pseudofermion phase shifts obey integral equations by their own. These equations read,

$$\Phi_{s_1, c_0}(r, r') = -\frac{1}{\pi} \arctan(r - r') + \int_{-r_0^c}^{r_0^c} dr'' G(r, r'') \Phi_{s_1, c_0}(r'', r') ,$$  
(A1)

$$\Phi_{s_1, c_\nu}(r, r') = -\frac{1}{\pi^2} \int_{-r_0^c}^{r_0^c} dr'' \arctan\left(\frac{r'' - r'}{\nu}\right) \int_{-r_0^c}^{r_0^c} dr'' G(r, r'') \Phi_{s_1, c_\nu}(r'', r') ,$$  
(A2)

and

$$\Phi_{s_1, s_\nu}(r, r') = \frac{\delta_{1, \nu}}{\pi} \arctan\left(\frac{r - r'}{2}\right) + \left(1 - \frac{\delta_{1, \nu}}{2}\right) \left\{ \frac{1}{\nu - 1} \arctan\left(\frac{r - r'}{\nu - 1}\right) + \frac{1}{\nu + 1} \arctan\left(\frac{r - r'}{\nu + 1}\right) \right\}$$
$$- \frac{1}{\pi^2} \int_{-r_0^c}^{r_0^c} dr'' \arctan\left(\frac{r'' - r'}{\nu}\right) \int_{-r_0^c}^{r_0^c} dr'' G(r, r'') \Phi_{s_1, s_1}(r'', r') .$$  
(A3)

Here the kernel $G(r, r')$ is given by [17],

$$G(r, r') = -\frac{1}{2\pi} \left[ \frac{1}{1 + ((r - r')/2)^2} \left(1 - \frac{1}{2} \left( t(r) + t(r') + \frac{l(r) - l(r')}{r - r'} \right) \right) \right] ,$$  
(A4)

where $t(r) = \frac{1}{2} \left[ \arctan(r + r_0^c) - \arctan(r - r_0^c) \right]$ and $l(r) = \frac{1}{2} [\ln(1 + (r + r_0^c)^2) - \ln(1 + (r - r_0^c)^2)]$. A second group of two-pseudofermion phase shifts are expressed in terms of the basic functions given in Eqs. [A1]-[A3] as follows,

$$\Phi_{c_0, c_0}(r, r') = \frac{1}{\pi} \int_{-r_0^c}^{r_0^c} dr'' \Phi_{s_1, c_0}(r'', r') \frac{1}{1 + (r - r'')^2} ,$$  
(A5)

$$\Phi_{c_0, c_\nu}(r, r') = -\frac{1}{\pi} \arctan\left(\frac{r - r'}{\nu}\right) + \frac{1}{\pi} \int_{-r_0^c}^{r_0^c} dr'' \Phi_{s_1, c_\nu}(r'', r') \frac{1}{1 + (r - r'')^2} ,$$  
(A6)
and

$$\tilde{\Phi}_{c, sv}(r, r') = -\frac{1}{\pi} \arctan\left(\frac{r - r'}{\nu}\right) + \frac{1}{\pi} \int_{-r_0^c}^{r_0^c} dr'' \frac{\Phi_{s, sv}(r'', r')}{1 + (r - r'')^2}. \quad (A7)$$

Finally, the remaining two-pseudofermion phase shifts can be expressed either in terms of the functions \([A6]-[A7]\) only,

$$\tilde{\Phi}_{c, c0}(r, r') = \frac{1}{\pi} \arctan\left(\frac{r - r'}{\nu}\right) - \frac{1}{\pi} \int_{-r_0^c}^{r_0^c} dr'' \frac{\Phi_{c, c0}(r'', r')}{\nu[1 + (r'' - \nu)]^2}, \quad (A8)$$

$$\tilde{\Phi}_{c, c\nu'}(r, r') = \frac{1}{2\pi} \Theta_{\nu, \nu'}(r - r') - \frac{1}{\pi} \int_{-r_0^c}^{r_0^c} dr'' \frac{\Phi_{c, c\nu'}(r'', r')}{\nu[1 + (r'' - \nu)]^2}, \quad (A9)$$

and

$$\tilde{\Phi}_{s, s\nu}(r, r') = \frac{1}{\pi} \int_{-r_0^c}^{r_0^c} dr'' \frac{\Phi_{s, c0}(r'', r')}{\nu[1 + (r'' - \nu)]^2}, \quad (A10)$$

or both in terms of the basic functions \([A1]-[A3]\) and of the phase shifts \([A5]-[A7]\),

$$\tilde{\Phi}_{s, c0}(r, r') = \frac{\arctan\left(\frac{r - r'}{\nu}\right)}{\pi} + \frac{1}{\pi} \int_{-r_0^c}^{r_0^c} dr'' \frac{\Phi_{s, c0}(r'', r')}{\nu[1 + (r'' - \nu)]^2} - \int_{-r_0^c}^{r_0^c} dr'' \Phi_{s, c0}(r'', r') \frac{\Theta_{\nu, 1}(r - r'')}{2\pi}; \quad \nu > 1, \quad (A11)$$

$$\tilde{\Phi}_{s, c\nu'}(r, r') = \frac{1}{\pi} \int_{-r_0^c}^{r_0^c} dr'' \frac{\Phi_{s, c\nu'}(r'', r')}{\nu[1 + (r'' - \nu)]^2} - \int_{-r_0^c}^{r_0^c} dr'' \Phi_{s, c\nu'}(r'', r') \frac{\Theta_{\nu, 1}(r - r'')}{2\pi}; \quad \nu > 1, \quad (A12)$$

and

$$\tilde{\Phi}_{s, s\nu}(r, r') = \frac{\Theta_{\nu, \nu'}(r - r')}{2\pi} + \frac{1}{\pi} \int_{-r_0^c}^{r_0^c} dr'' \frac{\Phi_{s, s\nu}(r'', r')}{\nu[1 + (r'' - \nu)]^2} - \int_{-r_0^c}^{r_0^c} dr'' \Phi_{s, s\nu}(r'', r') \frac{\Theta_{\nu, 1}(r - r'')}{2\pi}; \quad \nu > 1. \quad (A13)$$

In the above two-pseudofermion phase shift expressions the functions \(\Theta_{\nu, \nu'}(x)\) and \(\Theta_{\nu, 1}(x)\) are given in Eqs. (B5) and (C22) of Ref. \[27\], respectively. In spite of the different notation and except for simplifications introduced here as a result of some integrations performed analytically, the integral equations \([A1]-[A13]\) are equivalent to the system of coupled integral equations (B30)-(B40) of Ref. \[33\].

**APPENDIX B: THE \(\alpha\nu\) PSEUDOPARTICLE - PSEUDOFERMION UNITARY OPERATOR**

Here we confirm that in the PS the \(\alpha\nu\) pseudoparticle - pseudofermion operator \(\hat{V}_{\alpha\nu}\) that obeys Eq. (22) is unitary and given by expression \[23\]. While that expression refers to the PS, for any energy eigenstate of the full Hilbert space there is a one-to-one correspondence between the set of specific discrete values of the rapidity momentum \(\{k_j\} = \{k(q_j)\}\) such that \(j = 1, ..., N\) and the set of \(c0\) band discrete bare-momentum values \(\{q_j\}\). Moreover, there is a one-to-one correspondence between the set of specific discrete values of each \(\alpha\nu\)-branch \(\{\Lambda_{\alpha\nu}(q_j)\}\) such that \(j = 1, ..., N_{\alpha\nu}\) and the set of \(\alpha\nu\) band discrete bare-momentum values \(\{q_j\}\). These branches are such that \(\alpha = c, s\) and \(\nu = 1, 2, 3, ...\). This correspondence is fully defined by the integral equations (13)-(16) of Ref. \[23\], which refer to a functional representation of the thermodynamic Bethe-ansatz equations introduced by Takahashi \[20\]. The rapidity-momentum functional is real and the rapidity functionals are the real part of Takahashi’s ideal strings \[20, 23\].
Two alternative equivalent and complete descriptions for each energy eigenstate correspond to: (a) occupancy configurations of the above sets of discrete bare-momentum values \( \{q_j\} \) for the \( \alpha \nu \) bands with finite bare-momentum occupancy for the state plus occupancies of the \( L_{c,-1/2} \) and \( L_{s,-1/2} \) numbers; (b) occupancy configurations of the above set of discrete numbers \( \{k_j\} \) and \( \{\Lambda_{\alpha \nu}(q_j)\} \) for the \( \alpha \nu \) branches with finite occupancy of these numbers for the state plus occupancies of the \( L_{c,-1/2} \) and \( L_{s,-1/2} \) numbers. Since both these descriptions describe the same energy eigenstates, there is a uniquely defined transformation connecting the two alternative representations. That transformation refers to the whole Hilbert space.

For the PS, that correspondence assumes the simple form given in Eq. (18). There \( k^0(q_j) \) and \( \Lambda^0_{\alpha \nu}(q_j) \) are the initial ground-state rapidity-momentum and rapidity functions, respectively, whose inverse functions are given in Ref. [28] and \( \tilde{q}(q) \) is the canonical-momentum provided in Eq. (13). It follows from Eq. (18) that for the PS the \( \alpha \nu \) pseudoparticle - \( \alpha \nu \) pseudofermion transformation described by Eqs. (16) and (22) fully controls the above bare-momentum - rapidity-momentum/rapidity transformation. Since the \( \alpha \nu \) pseudoparticle - pseudofermion transformation connects two alternative representations for the complete set of orthogonality and normalized energy eigenstates that span the PS, the operator \( \hat{V}_{\alpha \nu} \) of Eq. (22) must be unitary in the PS, as confirmed below.

Equation (22) leads to,

\[
\hat{V}_{\alpha \nu}^\dagger = \exp\left\{ \sum_{q_j} \left[ b_{q_j+\delta(q_j), \alpha \nu} - b_{q_j, \alpha \nu}^\dagger \right] b_{q_j, \alpha \nu} \right\}; \quad \delta(q_j) = Q_{\alpha \nu}(q_j)/L .
\] (B1)

For the PS, the functional \( \delta(q_j) = Q_{\alpha \nu}(q_j)/L \) given in Eq. (14) is of the order \( 1/L \). Thus, within the thermodynamic limit that the pseudofermion description corresponds to, we use the following representation for the operator \( \left[ b_{q_j+\delta(q_j), \alpha \nu} - b_{q_j, \alpha \nu}^\dagger \right] \) in terms of the continuum bare-momentum \( q \),

\[
\left[ b_{q_j+\delta(q_j), \alpha \nu} - b_{q_j, \alpha \nu}^\dagger \right] = \delta(q) \frac{\partial}{\partial q} b_{q_j, \alpha \nu}^\dagger .
\] (B2)

Next, by expanding the exponential of Eq. (22) we find that to first-order in \( 1/L \) the operator (B1) obeys the following equation,

\[
\hat{V}_{\alpha \nu}^\dagger b_{q_j, \alpha \nu} = b_{q_j+\delta(q_j), \alpha \nu} \hat{V}_{\alpha \nu}^\dagger .
\] (B3)

This equation is equivalent to Eq. (B4). Therefore, this confirms that for the PS the operators (22) and (B1) indeed obey the relation (B2). Let us next show that in the PS these operators are unitary.

The operator (B1) can be rewritten as,

\[
\hat{V}_{\alpha \nu}^\dagger = e^{i\hat{G}_{\alpha \nu}} ; \quad \hat{G}_{\alpha \nu} = -i \sum_{q_j} \left[ b_{q_j+\delta(q_j), \alpha \nu}^\dagger - b_{q_j, \alpha \nu} \right] b_{q_j, \alpha \nu} .
\] (B4)

If the operator \( \hat{G}_{\alpha \nu} \) is hermitian then the operator \( \hat{V}_{\alpha \nu} \) is unitary. Let us show that the invariance of the \( \alpha \nu \) pseudoparticle number operator (30) under the transformation (16), which implies that it equals the \( \alpha \nu \) pseudofermion number operator (31), also implies the hermitian character of the operator \( \hat{G}_{\alpha \nu} \) of Eq. (B4).

Taking the transpose of the operator \( \hat{G}_{\alpha \nu} \) of Eq. (B4) leads to,

\[
\hat{G}_{\alpha \nu}^\dagger = i \sum_{q_j} b_{q_j, \alpha \nu}^\dagger \left[ b_{q_j+\delta(q_j), \alpha \nu} - b_{q_j, \alpha \nu} \right] .
\] (B5)

By using the transpose of Eq. (16) we rewrite the operator (B5) as,

\[
\hat{G}_{\alpha \nu}^\dagger = i \frac{L}{2\pi} \int dq \delta(q) \frac{\partial}{\partial q} \hat{G}_{\alpha \nu} b_{q, \alpha \nu} = -i \frac{L}{2\pi} \int dq \frac{\partial}{\partial q} \left[ \delta(q) b_{q, \alpha \nu}^\dagger \right] b_{q, \alpha \nu} + i \frac{L}{2\pi} \int dq \frac{\partial}{\partial q} \left[ \delta(q) b_{q, \alpha \nu}^\dagger b_{q, \alpha \nu} \right] = \hat{G}_{\alpha \nu}^\dagger - i \frac{L}{2\pi} \int dq \left[ \delta(q) b_{q, \alpha \nu}^\dagger b_{q, \alpha \nu} + i \frac{L}{2\pi} \int dq \frac{\partial}{\partial q} \left[ \delta(q) b_{q, \alpha \nu}^\dagger b_{q, \alpha \nu} \right] .
\] (B6)
where

$$
\hat{G}_{\alpha\nu} = -i \frac{L}{2\pi} \int dq \frac{\partial}{\partial q} \left[ \hat{b}^\dagger_{q,\alpha\nu} \right] b_{q,\alpha\nu} = -i \sum_{q_j} \left[ \hat{b}^\dagger_{q_j + \delta(q_j),\alpha\nu} - \hat{b}^\dagger_{q_j,\alpha\nu} \right] b_{q_j,\alpha\nu} .
$$

(B7)

In equations (B6) and (B6) we have replaced the bare-momentum summations by integrals over the whole $q$ domain of the corresponding $\alpha\nu$ band.

We emphasize that the operator $\hat{G}_{\alpha\nu}$ of Eq. (B4) is hermitian provided that the two last terms on the right-hand side of the last line of Eq. (B5) vanish. These terms can be rewritten as,

$$
-i \frac{L}{2\pi} \int dq \left[ \frac{\partial}{\partial q} \left( \delta(q) \right) \right] \hat{b}^\dagger_{q,\alpha\nu} b_{q,\alpha\nu} + i \frac{L}{2\pi} \int dq \frac{\partial}{\partial q} \left[ \delta(q) \hat{b}^\dagger_{q,\alpha\nu} b_{q,\alpha\nu} \right] 
$$

$$
= \frac{L}{2\pi} \int dq \delta(q) \left[ \frac{\partial}{\partial q} \left( \hat{b}^\dagger_{q,\alpha\nu} b_{q,\alpha\nu} \right) \right] - \frac{L}{2\pi} \int dq \frac{\partial}{\partial q} \left[ \delta(q) \hat{b}^\dagger_{q,\alpha\nu} b_{q,\alpha\nu} \right] + i \frac{L}{2\pi} \int dq \frac{\partial}{\partial q} \left[ \delta(q) \hat{b}^\dagger_{q,\alpha\nu} b_{q,\alpha\nu} \right] 
$$

$$
= i \sum_{q_j} \left[ \hat{N}_{\alpha\nu}(q_j + \delta(q_j)) - \hat{N}_{\alpha\nu}(q_j) \right] = i \left[ \sum_{q_j} \hat{N}_{\alpha\nu}(q_j) - \sum_{q_j} \hat{N}_{\alpha\nu}(q_j) \right] = i \left[ \hat{N}_{\alpha\nu} - \hat{\tilde{N}}_{\alpha\nu} \right] = 0 ,
$$

(B8)

where here the $\alpha\nu$ pseudofermion number operator (31) was called $\hat{N}_{\alpha\nu}$ and $\hat{\tilde{N}}_{\alpha\nu}$ is the $\alpha\nu$ pseudoparticle number operator (30). Since these operators are invariant under the transformation (10) they are the same operator, what justifies the vanishing of the operator terms. This shows that the operator $\hat{G}_{\alpha\nu}$ of Eq. (B4) is hermitian and thus that the operator $\hat{V}_{\alpha\nu}$ is unitary.

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