Scattering theories for the 1D Hubbard model

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In one-dimensional (1D) non-perturbative many-electron problems such as the 1D Hubbard model the electronic charge and spin degrees of freedom separate into exotic quantum objects. However, there are two different representations for such objects and associated scattering quantities whose relation is not well understood. Here we solve the problem by finding important information about the relation between the corresponding alternative choices for one-particle scattering states. Our study reveals why one of these representations, the pseudofermion representation, is the most suitable for the description of the unusual finite-energy spectral and dynamical properties of the model. This is a problem of physical importance, since the exotic independent charge and spin finite-energy spectral features observed by angle-resolved photoelectron spectroscopy in quasi-1D metals was found recently to correspond to the charge and spin quantum objects of the pseudofermion representation.

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1. INTRODUCTION

Recent photo-emission experiments in quasi-one-dimensional (1D) organic metals [1, 2, 3] have revealed finite-energy charge and spin spectral features similar to those predicted by the 1D Hubbard model, one of the few realistic electronic models for which all the energy eigenstates and their energies can be exactly calculated [4, 5]. In addition to describing quasi-1D organic metals the model can be experimentally realized with unprecedented precision in ultra-cold fermionic atomic systems and one may expect very detailed experimental results over a wide range of parameters to be available [6, 7].

In contrast to the model finite-energy physics, in the last fifteen years the low-energy behavior of correlation functions has been the subject of many studies [8, 9, 10, 11, 12, 13, 14]. Recently, the theoretical description of the experimentally observed finite-energy spectral features could be given using the pseudofermion dynamical theory (PDT), based on pseudofermionic accounting of the excitation spectrum [15, 16]. For example, the one-electron independent charge and spin spectral features experimentally observed for energies above the broken-symmetry states [17] in the metallic phase of low-dimensional organic compounds [1] correspond to power-law singularities along lines whose shape coincides with the energy dispersions of the charge and spin pseudofermion scatterers, respectively [18, 19]. Furthermore, the momentum and energy dependence of the corresponding spectral-weight distributions is fully controlled by the pseudofermion scattering [17, 18]. Also other exotic properties of the model were experimentally observed in low-dimensional complex materials [20, 21].

Another accounting of the elementary-excitation scattering quantities was given in Refs. [22, 23, 24]. While the latter description, based on spinon-holon accounting, was used in many theoretical studies of electronic correlated systems, its relation to the finite-energy spectral and dynamical properties is not well understood. The main goal of this paper is the clarification of the relation between the two scattering theories, of Refs. [18, 19] and Refs. [22, 23, 24], respectively, for the 1D Hubbard model, in view with the application of the former approach to dynamical calculations.

We begin by briefly reviewing the two approaches. The spin 1/2 spinon and the holon representation used in Refs. [22, 23, 24] was first introduced for the chiral invariant Gross-Neveu Hamiltonian [25], a continuum version of the Hubbard Hamiltonian. The spin 1/2 spinon corresponds to the color spin 1/2 particle of charge zero, whereas the massless excitation of that reference describes a quantum object associated with the charge degrees of freedom, now termed holon. The same excitation structure, decoupled spinon and holon was found for the Kondo model [26]. Subsequently, the same spinon - spin 1/2 spin wave representation was discussed [27] for the isotropic Heisenberg model. The reason for the same spin excitation structures in these models is that in each case their dynamics is based on a spin exchange interaction, $\vec{S} \cdot \vec{S}'$, leading to spin Bethe-ansatz (BA) equations that are isomorphic, differing only in their energy functions (and in their charge structure). Hence, the spin excitations possess the same quantum
numbers and the same scattering matrices. The charge excitations, on the other hand, differ in the various models and in particular in the Hubbard model, the holons acquire a \( \eta = 1/2 \) quantum number, associated with a charge \( SU(2) \) group.

While the spinons and holons of the conventional spinon-holon representation of Refs. were introduced by direct association with specific occupancy configurations of the quantum numbers of the BA solution, the pseudofermion description, used below, corresponds to occupancy configurations of “rotated electrons”, related to the original electron by a unitary transformation, chosen so that the states are characterized by their double occupancy. The pseudofermion description also refers to well defined occupancy configurations of the quantum numbers of the BA solution and the \( \eta \)-spin and spin \( SU(2) \) symmetries. Its choice of the objects whose occupancy configurations describe the energy eigenstates profits from the transformation laws under the electron - rotated-electron unitary transformation. Indeed, within the pseudofermion theory a well defined set of \( \eta \)-spin 1/2 holons and spin 1/2 spinons called Yang holons and HL spinons (Heilmann-Lieb spinons), respectively, are invariant under that transformation. As a result of that invariance such objects are neither scatterers nor scattering centers. All pseudofermion branches except one are closely related to the \( \eta \)-spin 1/2 holons or spin 1/2 spinons introduced in Ref. in terms of rotated-electron occupancies, which are different from those of the conventional spinon-holon representation of Refs., as further discussed in future sections of this paper. Indeed, the remaining holonic and spinonic degrees of freedom beyond the above Yang holons and HL spinons give rise to \( \eta \)-spin-zero 2\( \nu \)-holon composite charge \( c\nu \) pseudofermions and spin-zero \( s\nu \) 2\( \nu \)-spin composite pseudofermions, respectively, where \( \nu = 1, 2, 3, \ldots \). Finally, the energy eigenstates also involve occupancy configurations of charge \( c \) or c0 pseudofermions, which are independent of the holonic and spinonic degrees of freedom and thus are \( \eta \)-spin-less and spin-less objects.

The pseudofermion scattering description is a good starting point for the derivation of dynamical properties by means of the PDT. There are three main reasons why that description is more adapted to the calculations of finite-energy spectral functions than the related but different representation of Refs. and the conventional spinon-holon representation of Refs. . First, the pseudofermion energy spectrum has no residual-interaction terms, in contrast to that of the related objects of Refs. . This is behind the factorization of the one- and two-electron spectral functions in terms of pseudofermion spectral functions. Second, the pseudofermion \( S \) matrix is a simple phase factor, whereas that of the holons and spinons of the conventional representation of Refs. is a matrix of dimension larger than one. Third, for the metallic phase all one-pseudofermion scattering states of the pseudofermion theory correspond to many-pseudofermion energy eigenstates, whereas some of the alternative spinon-holon scattering states of the theory of Refs. do not refer to energy eigenstates. As further discussed in Sec. IV-B, the second and third points considerably simplify the calculation of the finite-energy spectral functions, when expressed in terms of Lehmann representations.

The pseudofermion theory is a generalization for finite values of the on-site repulsion \( U \) of the \( U/t >> 1 \) method introduced in Ref. , where \( t \) is the first-neighbor transfer integral. The natural excitation basis that arises for \( U/t >> 1 \) is the one considered in the studies of Refs. for all values of \( U/t \). For instance, the spin-less fermions of Refs., the spins or spinons of Refs., and the doublons and holons of Ref. correspond to the c0 pseudofermions, spinons, and \( \eta \)-spin projection \( -1/2 \) and \( +1/2 \) holons, respectively, of Refs. for \( U/t >> 1 \). The studies of Ref. confirm that in the limit of low energy the finite-energy PDT reproduces the well known results and behaviors of the spectral and correlation functions previously obtained by use of conformal-field theory and bosonization.

Here we show that both the representations are faithful and correspond to two different choices of one-particle scattering states and thus that there is no inconsistency between the two corresponding definitions of scatterers and scattering centers. Moreover, we complete the preliminary analysis of Ref. and confirm that the pseudofermion representation is the most suitable for the description of the finite-energy spectral and dynamical properties. Our results apply to other integrable interacting problems besides the 1D Hubbard model and therefore have wide applicability.

Concerning the conventional spinon-holon representation, in this paper we use the notation of Refs. . We note that in spite of using a different notation, the spinon-holon representation of Ref. is the same as that used in these references. The paper is organized as follows: In section II we introduce the 1D Hubbard model and summarize the basic information about the pseudofermion description needed for our investigations. In Sec. III we consider the pseudofermion scattering quantities and clarify the connection of the pseudofermion and pseudofermion-hole phase shifts and corresponding \( S \) matrices to the elementary-excitation phase shifts and \( S \) matrices, respectively, previously obtained in Refs. . In Sec. IV we extend the spinon-holon conventional scattering theory of Refs. to the larger Hilbert subspace of the pseudofermion scattering theory and confirm the faithful character of both quantum-object representations. Moreover, in that section we discuss the suitability for applications to the study of the finite-energy spectral and dynamical properties. Finally, Sec. V contains the concluding remarks.
II. THE 1D HUBBARD MODEL AND THE PSEUDOFERMION SCATTERING THEORY

In this section we introduce the 1D Hubbard model and summarize the concepts and results concerning the rotated electrons [28] and the pseudofermion description [15, 16, 30] that are needed for our studies.

The basic Hamiltonian, defined on a 1D lattice with \( N_a \) sites, is given by,

\[
\hat{H} = -t \sum_{j=1}^{N_a} (c_{j,\sigma}^\dagger c_{j+1,\sigma} + \text{h.c.}) + U \sum_{j=1}^{N_a} n_{j\uparrow} n_{j\downarrow} \equiv \hat{T} + U \hat{D},
\]

where, the operator \( c_{j,\sigma} \) (and \( c_{j,\sigma}^\dagger \)) creates (and annihilates) a spin-projection \( \sigma \) electron at lattice site \( j = 1, 2, ..., N_a \), \( \hat{n}_{j,\sigma} = c_{j,\sigma}^\dagger c_{j,\sigma} \) counts the number of spin-projection \( \sigma \) electrons at lattice site \( j \), \( \hat{T} = -t \sum_{\sigma=\uparrow,\downarrow} \sum_{j=1}^{N_a} [c_{j,\sigma}^\dagger c_{j+1,\sigma} + \text{h.c.}] \) is the kinetic-energy operator, and \( \hat{D} = \sum_{j=1}^{N_a} \hat{n}_{j,\uparrow} \hat{n}_{j,\downarrow} \) is the electron double-occupation operator.

The model has an obvious \( U(1) \times SU(2) \) symmetry,

\[
\begin{align*}
    c_{j,\sigma} &\rightarrow \ e^{i\theta} c_{j,\sigma}, \\
    c_{j,\sigma} &\rightarrow \ U_{\sigma,\sigma'} c_{j,\sigma'},
\end{align*}
\]

expressing the charge conservation and invariance under spin rotation. The associated generators are given by the number operator,

\[
\hat{N} = \sum_{j=1}^{N_a} (\hat{n}_{j\uparrow} + \hat{n}_{j\downarrow}),
\]

and the spin operators,

\[
S_\sigma^z = \frac{1}{2} \sum_{j=1}^{N_a} (\hat{n}_{j\uparrow} - \hat{n}_{j\downarrow}), \quad S_\sigma^+ = \sum_{j=1}^{N_a} c_{j,\uparrow}^\dagger c_{j,\uparrow}, \quad S_\sigma^- = (S_\sigma^+)^* ,
\]

respectively. There is another (less obvious) charge \( SU(2) \) invariance present in a slightly modified version of the model [28],

\[
\hat{H}_H = -U \sum_{j=1}^{N_a} \left( \hat{n}_{j\downarrow} + \hat{n}_{j\uparrow} - \frac{1}{2} \right),
\]

where a chemical potential \( U/2 \) term was added to the Hamiltonian. In a grand canonical ensemble the model will be half filled. Equivalently, the symmetry will show up if we work in the canonical ensemble and choose the filling appropriately. The symmetry is realized by number density and pair creation and annihilation operators,

\[
S_c^z = \frac{1}{2} \sum_{j=1}^{N_a} (n_{j\uparrow} + n_{j\downarrow} - 1), \quad S_c^+ = \sum_{j=1}^{N_a} (-1)^j c_{j,\downarrow}^\dagger c_{j,\uparrow}, \quad S_c^- = (S_c^+)^* .
\]

As the number operator does not commute with \( S_c^\pm \), the symmetry manifests itself only upon comparing excitations in systems with different number of electrons. For historical reasons we refer to the charge \( SU(2) \) as \( \eta \)-spin [28]. Adding a chemical potential \( \mu \) and magnetic field \( H \) the Hamiltonian takes the form,

\[
\hat{H} = \hat{H}_{SO(4)} + \sum_{\alpha=c, s} \mu_\alpha \hat{S}_\alpha^z; \quad \hat{H}_{SO(4)} = \frac{U}{2} \left[ \hat{N} - \frac{N_a}{2} \right]; \quad \hat{H}_H = \hat{T} + U \hat{D},
\]

where \( \mu_c = 2\mu \), \( \mu_s = 2\mu_0 H \), and \( \mu_0 \) is the Bohr magneton. The momentum operator is given by \( \hat{P} = \sum_{\sigma=\uparrow,\downarrow} \sum_k \hat{n}_\sigma(k) k \), where the spin-projection \( \sigma \) momentum distribution operator reads \( \hat{n}_\sigma(k) = c_{k,\sigma}^\dagger c_{k,\sigma} \).

Throughout this paper we use units of both Planck constant \( h \) and lattice constant \( a \) one. We denote the electronic charge by \(-e\), the lattice length by \( L = N_a a = N_a \), and the \( \eta \)-spin value \( \eta \) (and spin value \( S \)) and \( \eta \)-spin projection \( \eta_z \) (and spin projection \( S_z \)) of the energy eigenstates by \( S_c \) and \( S_c^z \) (and \( S_s \) and \( S_s^z \)), respectively. For the description of the transport of charge in terms of electrons (and electronic holes), the Hamiltonians provided in Eq. (6) describe
pseudofermion occupancy configurations describe the BA charge distribution of pseudofermions for spin string excitations of length $SU(2)$ creation and annihilation operators. For instance, the $\eta$ unitary transformation. Indeed, the Yang holons and HL spinons are also invariant under that transformation $[29]$. An on-site electronic Cooper pair transforms $a + 1/2\alpha$ and HL spinon total numbers. However, all the Yang holons and HL spinons of the latter states have the same contained in that solution have precisely the same pseudofermion occupancies and the same Yang holon and spin projections, respectively. (For more information about Yang holons and HL spinons see Sec. 2.4 of Ref. $[29]$.)

The $c\eta$ pseudofermions have no spin and $\eta$-spin degrees of freedom. The $cv$ pseudofermions for $\nu > 0$ (and $sv$ pseudofermions), are composite objects having $\eta$-spin zero (and spin zero) consisting of an equal number $\nu = 1, 2, ...$ of $-1/2$ holons and $+1/2$ holons (and $-1/2$ spinons and $+1/2$ spinons). In this paper we use the notation $a\nu$ pseudofermion, where $\alpha = c, s$ and $\nu = 0, 1, 2, ...$ for the $cv$ branches and $\nu = 1, 2, ...$ for the $sv$ branches. As further discussed in Sec. IV-A, the holons, $c\eta$ pseudofermions, and composite $cv$ pseudofermions are charged objects. The different pseudofermion branches correspond to well known types of BA excitations. For instance, in the $c\eta$ pseudofermion occupancy configurations describe the BA charge distribution of $k's$ excitations and those of the $cv$ pseudofermions for $\nu > 0$ (and $sv$ pseudofermions) describe the BA charge string excitations of length $\nu$ (and BA spin string excitations of length $\nu$).

The properties of the Yang holons and HL spinons follow from the invariance of the three generators of the $\eta$-spin $SU(2)$ algebra and three generators of the spin $SU(2)$ algebra, respectively, under the electron - rotated-electron unitary transformation. Indeed, the Yang holons and HL spinons are also invariant under that transformation $[29]$. Therefore, the operators that transform such objects have the same form in terms of electronic and rotated-electron creation and annihilation operators. For instance, the $\eta$-spin off diagonal generator that creates (and annihilates) an on-site electronic Cooper pair transforms $a + 1/2$ Yang holon and $a - 1/2$ Yang holon (and $a + 1/2$ Yang holon). Furthermore, the spin off diagonal generator that flips an on-site electronic up spin (and down spin) onto an on-site electronic down spin (and up spin) also transforms a $+1/2$ HL spinon (and $-1/2$ HL spinon) into a $-1/2$ HL spinon (and $+1/2$ HL spinon). Thus, the occupancies of these objects involving Yang holons with different $\eta$-spin projections $+1/2$ and $-1/2$ and/or HL spinons with different spin projections $+1/2$ and $-1/2$ describe the energy eigenstates that are not contained the BA solution. The corresponding energy eigenstates contained in that solution have precisely the same pseudofermion occupancy configurations and the same Yang holon and HL spinon total numbers. However, all the Yang holons and HL spinons of the latter states have the same $\eta$-spin and spin projections, respectively. (For more information about Yang holons and HL spinons see Sec. 2.4 of Ref. $[29]$.)

We denote the number of $a\nu$ pseudofermions by $N_{a\nu}$ and the number $\pm 1/2$ Yang holons ($\alpha = c$) and $\pm 1/2$ HL spinons ($\alpha = s$) by $L_{\alpha, \pm 1/2}$. As mentioned above, besides corresponding to well defined occupancies of the BA quantum numbers, the holons, spinons, and pseudofermions can also be expressed in terms of rotated electrons. For instance, $N_{c\eta}$ equals the number of rotated-electron singly occupied sites and $[N_a - N_{c\eta}]$ equals the number of rotated-electron doubly occupied plus unoccupied sites. We call $M_{\alpha, \pm 1/2}$ the number of $\pm 1/2$ holons ($\alpha = c$) and $\pm 1/2$ spinons ($\alpha = s$). The latter number and that of $\pm 1/2$ Yang holons ($\alpha = c$) and $\pm 1/2$ HL spinons ($\alpha = s$) are given by $M_{\eta, \pm 1/2} = L_{\eta, \pm 1/2} + \sum_{\nu = 1}^{\infty} \nu N_{a\nu}$ and $L_{\eta, \pm 1/2} = S_{\eta} + S_{\eta}$. Within the pseudofermion, Yang holon, and HL spinon description the energy and momentum spectrum of the PS energy eigenstates has the form provided in Eqs. (28)-(34) of Ref. $[17]$. Such a spectrum is expressed in terms of the pseudofermion energy dispersions defined in Eqs. (C.15)-(C.18) of Ref. $[29]$, pseudofermion bare-momentum distribution-function deviations given in Eqs. (13)-(17) of Ref. $[15]$, and Yang holon ($\alpha = c$) and HL spinon ($\alpha = s$) occupancies $L_{\alpha, \pm 1/2} = S_{\alpha} + S_{\alpha}$. (The pseudofermion energy dispersions equal those plotted in Figs. 6-9 of Ref. $[32]$.) As explained in detail in Ref. $[29]$, the number of $\pm 1/2$ holons and $\pm 1/2$ spinons can be expressed in terms of the
number \( N_\sigma \) of spin-projection \( \sigma \) electrons and rotated electrons, \( N^h = [2N_\sigma - N] \) of electronic holes and rotated-electron holes, and \( N_{c\sigma} \) of rotated-electron singly occupied sites as \( M_{c\sigma} - 1/2 = [N - N_{c\sigma}] / 2 \), \( M_{c\sigma} + 1/2 = [N^h - N_{c\sigma}] / 2 \), and \( M_{c\sigma} + 1 = [N_\sigma + N_c - N_\sigma] / 2 \). We recall that the number \( N_{c\sigma} \) of rotated-electron singly occupied sites also equals the number \( c\sigma \) pseudofermions and the number \([N_\sigma - N_{c\sigma}]\) of rotated-electron doubly-occupied and unoccupied sites equals that of \( c\sigma \) pseudofermion holes. Furthermore, \( M_\sigma = [M_{c\sigma} - 1/2 + M_{c\sigma} + 1/2] \) denotes the number of holons \( (\alpha = c) \) or spinons \( (\alpha = s) \) such that \( M_c = [N_\sigma - N_{c\sigma}] \) and \( M_s = N_{c\sigma} \) and \( L_\sigma = [L_{c\sigma} - 1/2 + L_{c\sigma} + 1/2] \) denotes the number of Yang holons \( (\alpha = c) \) or IL spinons \( (\alpha = s) \) such that \( L_c = 2S_c = 2\eta \) and \( L_s = 2S_s = 2\eta \). Often in this paper we use the notation \( \alpha\nu \neq c, s \) branches, which refers to all \( \alpha\nu \) branches except the \( c\sigma \) and \( s\sigma \) branches. Moreover, the summation (and product) \( \sum_{\alpha\nu} \) (and \( \prod_{\alpha\nu} \)) runs over all \( \alpha\nu \) branches with finite \( \alpha\nu \) pseudofermion occupancy in the corresponding state or subspace and the summation \( \sum_{\alpha} \) runs over \( \alpha = c, s \). An important point for our studies is that for a ground state with densities in the ranges considered in this paper the above numbers read \( N_\sigma = N, N_{s\uparrow} = N_{\downarrow}, M_{c\uparrow} + 1/2 = L_{c\uparrow} + 1/2 = [N_\sigma - N], M_{c\downarrow} - 1/2 = N_{\downarrow}, M_{c\downarrow} + 1/2 = N_{\uparrow}, L_{c\uparrow} + 1/2 = [N_{\uparrow} - N_{\downarrow}], \) and \( N_{\alpha\nu} = M_{c\sigma} - 1/2 = L_{c\sigma} - 1/2 = 0 \) for \( \alpha\nu \neq c, s \) and \( \alpha = c, s \).

The \( \alpha\nu \) pseudofermion discrete canonical-momentum values \( \tilde{q}_j \) are of the following form,

\[
\tilde{q}_j = \tilde{q}(q_j) = q_j + \frac{Q^{c\nu}(q_j)}{L} = \frac{2\pi}{L} I_j^{\alpha\nu} + \frac{Q^{c\nu}(q_j)}{L}; \quad j = 1, 2, \ldots, N_{\alpha\nu}^c.
\]

Here \( I_j^{\alpha\nu} \) are the actual quantum numbers which are integers or half-odd integers \(^{30}\) and the discrete bare-momentum \( q_j \) such that \( q_{j+1} - q_j = 2\pi / L \) has allowed occupancies one and zero only. The corresponding discrete canonical-momentum \( \tilde{q}_j \) such that \( \tilde{q}_{j+1} - \tilde{q}_j = 2\pi / L + 1/(L^2) \) has also allowed occupancies one and zero only. The bare-momentum distribution function \( N_{\alpha\nu}(q_j) \) is such that \( N_{\alpha\nu}(q_j) = 1 \) for occupied bare-momentum values and \( N_{\alpha\nu}(q_j) = 0 \) for unoccupied bare-momentum values. We denote the ground-state bare-momentum distribution function by \( N_{\alpha\nu}^0(q_j) \). It is given in Eqs. (C.1)-(C.3) of Ref. \(^{29}\). Except for \( 1/L \) corrections, for initial ground states with densities in the ranges considered here the \( c\sigma \) and \( s\sigma \) pseudofermion Fermi momentum values \( \pm q_{kF}^{c\nu} \) and limiting bare-momentum values \( \pm q_{kF}^{c\nu} \) of the \( \alpha\nu \) band are such that,

\[
q_{kF}^{c\nu} = 2k_F; \quad q_{kF}^{c\uparrow} = \pi; \quad q_{kF}^{c\downarrow} = 0; \quad q_{kF}^{c\nu} = |k_{F\uparrow} - k_{F\downarrow}|, \quad \nu > 0.
\]

For the PS where the pseudofermion representation is defined, the set of limiting values given in Eq. \(^{33}\) also gives the corresponding canonical-momentum limiting values, which remain unchanged for the excited states \(^{19}\). (The ground-state Fermi bare-momentum values and limiting bare-momentum values including the \( 1/L \) corrections are given in Eqs. (C.4)-(C.11) and (B.14)-(B.17), respectively, of Ref. \(^{22}\).)

A \( \alpha\nu \) pseudofermion can be labeled by the bare-momentum \( q_j \) or corresponding canonical momentum \( \tilde{q}_j \). Indeed, there is a one-to-one correspondence between the bare momentum \( q_j \) and the canonical momentum \( \tilde{q}_j = q_j + Q^{c\nu}(q_j) / L \) for \( j = 1, 2, \ldots, N_{\alpha\nu} \). A \( \alpha\nu \) pseudofermion (and \( \alpha\nu \) pseudofermion hole) of bare-momentum \( q_j \) corresponds to an occupied (and unoccupied) BA quantum number \( I_j^{c\nu} \) of Eq. \(^{7}\). The above number \( N_{\alpha\nu}^c \) is such that \( N_{\alpha\nu} = N_{\alpha\nu}^c + N_{\alpha\nu}^0 \) where \( N_{\alpha\nu}^0 \) denotes the number of \( \alpha\nu \) pseudofermion holes. (The expression of \( N_{\alpha\nu}^0 \) is given in Eqs. (B.7) and (B.8) of Ref. \(^{21}\).) Note that besides equalling the number of discrete canonical-momentum values in the \( \alpha\nu \) band, \( N_{\alpha\nu}^c \) also equals the number of sites of the \( \alpha\nu \) effective lattice \(^{31}\) which plays an important role in the pseudofermion description. In addition to the \( \alpha\nu \) pseudofermions of canonical momentum \( \tilde{q}_j \), there are local \( \alpha\nu \) pseudofermions, whose creation and annihilation operators correspond to the sites of the effective \( \alpha\nu \) lattice. Such a lattice has spatial coordinates \( x_j = a_{\alpha\nu} j \) where \( a_{\alpha\nu} = L / N_{\alpha\nu} \) is the effective \( \alpha\nu \) lattice constant and \( j = 1, 2, \ldots, N_{\alpha\nu} \). Each \( \alpha\nu \) pseudofermion band is associated with an effective \( \alpha\nu \) lattice whose length \( L = N_{\alpha\nu} \) is the same as that of the original real-space lattice. The canonical-momentum pseudofermion operators and local pseudofermion operators are related by a Fourier transform \(^{30}\).

The canonical-momentum shift functional \( Q^{c\nu}(q_j) / L \) appearing in the canonical-momentum expression \(^{7}\) is given by,

\[
Q^{c\nu}(q_j) / L = \frac{2\pi}{L} \sum_{\alpha\nu'} N_{\alpha\nu'} \sum_{j' = 1}^{N_{\alpha\nu'}} \Phi_{\alpha\nu', \alpha\nu'}(q_j, q_{j'}) \Delta N_{\alpha\nu'}(q_{j'}),
\]

where \( \Delta N_{\alpha\nu}(q_{j'}) = N_{\alpha\nu}(q_{j'}) - N_{\alpha\nu}^0(q_{j'}) \) is the \( \alpha\nu \) bare-momentum distribution-function deviation. Thus, \( \tilde{q}_j = q_j \) for the initial ground state. A PS excited energy eigenstate is uniquely defined by the values of the set of deviations \( \{\Delta N_{\alpha\nu}(q_{j'})\} \) for all values of \( q_{j'} \) corresponding to the \( \alpha\nu \) branches with finite pseudofermion occupancy in the state and by the values \( L_{c\sigma} - 1/2 \) and \( L_{c\sigma} + 1/2 \). The quantity \( \Phi_{\alpha\nu', \alpha\nu'}(q, q') \) on the right-hand side of Eq. \(^9\) is a function of both the bare-momentum values \( q \) and \( q' \) given by,

\[
\Phi_{\alpha\nu, \alpha'\nu'}(q, q') = \Phi^{c\nu, c\nu'}_{\alpha\nu, \alpha'\nu'} \left( \frac{4\pi A_0^0(q)}{U}, \frac{4\pi A_0^0(q')}{U} \right),
\]
where the function $\Phi_{\alpha\nu,\alpha'\nu'}(r, r')$ is the unique solution of the integral equations (A1)-(A13) of Ref. 30. The ground-state rapidity functions $\Lambda_{\alpha\nu}^0(q)$ appearing in Eq. 10, where $\Lambda_{\alpha\nu}^0(q) \equiv \sin k^0(q)$ for $\alpha\nu = c0$, are defined in terms of the inverse functions of $k^0(q)$ and $A_{\alpha\nu}^0(q)$ for $\nu > 0$ in Eqs. (A.1) and (A.2) of Ref. 13. As discussed below, $2\pi \Phi_{\alpha\nu,\alpha'\nu'}(q, q')$ or $-2\pi \Phi_{\alpha\nu,\alpha'\nu'}(q, q')$ is an elementary two-pseudofermion phase shift such that $q$ is the bare-momentum value of a $\alpha\nu$ pseudofermion or $\alpha'\nu'$ pseudofermion hole scattered by a $\alpha'\nu'$ pseudofermion hole $\nu$ of bare-momentum $q'$ created under a ground-state - excited-energy-eigenstate transition. For initial ground states with electronic density $n = 1$ (and spin density $m = 0$) and $\alpha'\nu' \neq c0$ or $\alpha'\nu' \neq c0$ branches (and $\nu \neq 1$ or $\nu' \neq 1$ branches), the ground-state rapidity function $\Lambda_{\alpha\nu}^0(q)$ or $\Lambda_{\alpha'\nu'}^0(q')$ appearing in expression 10 must be replaced by that of the excited state described by the bare-momentum distribution-function deviations on the right-hand side of Eq. 9.

III. S MATRICES AND PHASE SHIFTS

Here we consider the general pseudofermion and hole $S$ matrices and phase shifts. Moreover, we relate the phase shifts and $S$ matrices of the two representations mentioned in Sec. I for the reduced subspace considered in the studies of Refs. 23, 24.

A. PSEUDOFE RMI ON AND HOLE $S$ MATRICES

Our analysis refers to periodic boundary conditions and very large values of $L$. The PS energy and momentum eigenstates can be written as direct products of states spanned by the occupancy configurations of each of the $\alpha\nu$ branches with finite pseudofermion occupancy in the state under consideration. Moreover, the many-pseudofermion states spanned by occupancy configurations of each $\alpha\nu$ branch can be expressed as a direct product of $N^*_{\alpha\nu}$ one-pseudofermion states, each referring to one discrete bare-momentum value $q_j$, where $j = 1, 2, ..., N^*_{\alpha\nu}$. Within the pseudofermion description, the 1D Hubbard model in normal order relative to the initial ground state reads 30:

$$
\hat{H} := \sum_{\alpha\nu} \sum_{j=1}^{N^*_{\alpha\nu}} \hat{H}_{\alpha\nu,q_j} + \sum_{\alpha} \hat{H}_\alpha, \quad \text{where} \quad \hat{H}_{\alpha\nu,q_j} \quad \text{is the one-pseudofermion Hamiltonian which describes the} \quad \alpha\nu \quad \text{pseudofermion or hole of bare-momentum} \quad q_j \quad \text{and} \quad \hat{H}_\alpha \quad \text{refers to the Yang holons (}\alpha = c\text{) and HL spinons (}\alpha = s\text{). (As discussed below, the latter objects are scatter-less.) For each many-pseudofermion PS energy eigenstate the number of Hamiltonians} \quad \hat{H}_{\alpha\nu,q_j}, \quad \text{equals that of one-pseudofermion states given by,} \quad N^*_{\alpha} + N^*_1 + \sum_{\alpha\nu \neq c0} \theta(|\Delta N_{\alpha\nu}|) N^*_{\alpha\nu} \quad \text{where} \theta(x) = 1 \quad \text{for} \quad x > 0 \quad \text{and} \quad \theta(x) = 0 \quad \text{for} \quad x = 0 \quad \text{and the pseudofermion numbers refer to the energy eigenstate under consideration.}

The ground-state - excited-energy-eigenstate transitions can be divided into three steps. The first step refers to the ground-state - virtual-state transition. It is scatter-less and changes the number of discrete bare-momentum values of the $\alpha\nu \neq c0$ bands. Moreover, the first step involves the pseudofermion creation and annihilation processes and pseudofermion particle-hole processes associated with PS excited states. The second step is also scatter-less and generates the "in" state. Indeed, the one-pseudofermion states belonging to the many-pseudofermion "in" state are the "in" asymptote states of the pseudofermion scattering theory. The generator of the virtual-state - "in"-state transition is of the form $S^0 = \prod_{\alpha\nu} \prod_{j=1}^{N^*_{\alpha\nu}} S_{\alpha\nu,q_j}$, where $S_{\alpha\nu,q_j}$ is a well-defined one-pseudofermion unitary operator. Application of $S_{\alpha\nu,q_j}$ onto the corresponding one-pseudofermion state of the many-pseudofermion virtual state shifts its discrete bare-momentum value $q_j$ to the bare-momentum value $q_j + Q^0_{\alpha\nu}/L$, where $Q^0_{\alpha\nu}$ is given in Eq. A1 of Appendix A. Finally, the third step consists of a set of two-pseudofermion scattering events. It corresponds to the "in"-state - "out"-state transition, where the latter state is the PS excited energy eigenstate under consideration. The generator of that transition is the operator, $S^\phi = \prod_{\alpha\nu} \prod_{j=1}^{N^*_{\alpha\nu}} S^\phi_{\alpha\nu,q_j}$, where $S^\phi_{\alpha\nu,q_j}$ is a well-defined one-pseudofermion scattering unitary operator. The one-pseudofermion states belonging to the many-pseudofermion "out" state are the "out" asymptote pseudofermion scattering states. Application of $S^\phi_{\alpha\nu,q_j}$ onto the corresponding one-pseudofermion state of the many-pseudofermion "in" state shifts its discrete bare-momentum value $q_j + Q^0_{\alpha\nu}/L$ to the "out"-state discrete canonical-momentum value $q_j + Q_{\alpha\nu}(q_j)/L$, where

$$
Q_{\alpha\nu}(q_j) = Q^0_{\alpha\nu} + Q^\phi_{\alpha\nu}(q_j).
$$

We note that the generator of the virtual-state - "out"-state transition is the unitary operator $\hat{S} = \prod_{\alpha\nu} \prod_{j=1}^{N^*_{\alpha\nu}} \hat{S}_{\alpha\nu,q_j}$, where $\hat{S}_{\alpha\nu,q_j}$ is the one-pseudofermion or hole unitary $\hat{S}_{\alpha\nu,q_j} = \hat{S}^\phi_{\alpha\nu,q_j} S_{\alpha\nu,q_j}$ operator. The unitary $\hat{S}_{\alpha\nu,q_j}$ operator shifts the discrete bare-momentum value $q_j$ of the one-pseudofermion state belonging to the virtual state directly to the "out"-state discrete canonical-momentum value $q_j + Q_{\alpha\nu}(q_j)/L$. 


The virtual state, "in" state, and "out" state are PS energy eigenstates, as further discussed below. Thus, that the one-pseudofermion states of the many-pseudofermion "in" state and "out" state are the one-pseudofermion "in" and "out" asymptote scattering states, respectively, implies that the one-pseudofermion Hamiltonian \( \hat{H}_{\alpha\nu,q_j} \) plays the role of the unperturbed Hamiltonian \( \hat{H}_0 \) of the spin-less one-particle nonrelativistic scattering theory. Indeed, the unitary \( \hat{S}_{\alpha\nu,q_j} \) operator (and the scattering unitary \( \hat{S}_{\alpha\nu} \) operator) commutes with the Hamiltonian \( \hat{H}_{\alpha\nu,q_j} \) and thus the one-pseudofermion "in" and "out" asymptote scattering states are energy eigenstates of \( \hat{H}_{\alpha\nu,q_j} \) and eigenstates of \( \hat{S}_{\alpha\nu,q_j} \) (and \( \hat{S}_{\alpha\nu} \)). It follows that the matrix elements between one-pseudofermion states of \( \hat{S}_{\alpha\nu,q_j} \) (and \( \hat{S}_{\alpha\nu} \)) are diagonal and thus these operators are fully defined by the set of their eigenvalues belonging to these states. The same applies to the above generator \( \hat{S} \) (and \( \hat{S}^\Phi \)). The matrix elements of that generator between virtual states (and "in" states) are also diagonal and thus is fully defined by the set of its eigenvalues belonging to the virtual states (and "in" states). Since \( \hat{S}_{\alpha\nu,q_j} \) and \( \hat{S}_{\alpha\nu} \) are unitary, each of their eigenvalues has modulus one and can be written as the exponent of a purely imaginary number given by,

\[
\Phi_{\alpha\nu}(q_j) = e^{iQ_{\alpha\nu}(q_j)} = \prod_{\alpha'\nu'} N_{\alpha'\nu'}^{\alpha\nu} S_{\alpha\nu,\alpha'\nu'}(q_j, q_{j'}); \quad j = 1, 2, ..., N_{\alpha\nu}^*,
\]

\[
\Phi_{\alpha\nu}(q_j) = e^{iQ_{\alpha\nu}(q_j)} = e^{iQ_{\alpha\nu}^\Phi S_{\alpha\nu}^\Phi(q_j)}; \quad j = 1, 2, ..., N_{\alpha\nu}^*.
\]

Here \( Q_{\alpha\nu}^\Phi(q_j) \) and \( Q_{\alpha\nu}(q_j) \) are the functionals defined in Eqs. (10) and (11), respectively. By use of the former functional we find that,

\[
S_{\alpha\nu,\alpha'\nu'}(q_j, q_{j'}) = e^{i2\pi \Phi_{\alpha\nu,\alpha'\nu'}(q_j, q_{j'}) \Delta N_{\alpha'\nu'}(q_{j'})},
\]

where the functions \( \Phi_{\alpha\nu,\alpha'\nu'}(q_j, q_{j'}) \) are given in Eq. (10). The effect of under a ground-state - excited-energy-eigenstate transition moving the \( \alpha\nu \) pseudofermion or hole of initial ground-state canonical-momentum \( q_j = q_j \) once around the length \( L \) lattice ring is that its wave function acquires the overall phase factor \( S_{\alpha\nu}(q_j) \) given in Eq. (12). The phase factor \( S_{\alpha\nu,\alpha'\nu'}(q_j, q_{j'}) \) of Eq. (13) in the wave function of the \( \alpha\nu \) pseudofermion or hole results from a elementary two-pseudofermion zero-momentum forward-scattering event whose scattering center is a \( \alpha'\nu' \) pseudofermion (\( \Delta N_{\alpha'\nu'}(q_{j'}) = 1 \)) or \( \alpha'\nu' \) pseudofermion hole (\( \Delta N_{\alpha'\nu'}(q_{j'}) = -1 \)) created under the ground-state - excited-state transition. Thus, the third step of that transition involves a well-defined set of elementary two-pseudofermion scattering events where all \( \alpha\nu \) pseudofermions and \( \alpha\nu \) pseudofermion holes of bare-momentum \( q_j + Q_{\alpha\nu}^0/L \) of the "in" state are the scatterers, which leads to the overall scattering phase factor \( S_{\alpha\nu}^\phi(q_j) \) in their wave function provided in Eq. (12). That the scattering centers are the \( \alpha'\nu' \) pseudofermions or pseudofermion holes of momentum \( q_{j'} + Q_{\alpha\nu}^0/L \) created under the ground-state - excited-energy-eigenstate transition is confirmed by noting that \( S_{\alpha\nu,\alpha'\nu'}(q_j, q_{j'}) = 1 \) for \( \Delta N_{\alpha'\nu'}(q_{j'}) = 0 \). Thus, out of the scatterers whose number equals that of the one-pseudofermion states given above, the scattering centers are only those whose bare-momentum distribution-function deviation is finite. The elementary two-pseudofermion scattering processes associated with the phase factors (13) conserve the total energy and total momentum, are of zero-momentum forward-scattering type and thus conserve the individual "in" asymptote \( \alpha\nu \) pseudofermion momentum value \( q_j + Q_{\alpha\nu}^0/L \) and energy, and also conserve the \( \alpha\nu \) branch, usually called channel in the scattering language. Moreover, the scattering amplitude does not connect quantum objects with different \( \eta \) spin or spin.

Importantly, for each \( \alpha\nu \) pseudofermion or pseudofermion hole of virtual-state bare-momentum \( q_j \), the \( S \) matrix associated with the ground-state - excited-energy-eigenstate transition is simply the phase factor \( S_{\alpha\nu}(q_j) \) given in Eq. (12). Application of the unitary \( \hat{S}_{\alpha\nu,\alpha'\nu'} \) operator onto its one-pseudofermion state of the many-pseudofermion virtual state generates the corresponding one-pseudofermion state of the many-pseudofermion "out" state. The latter one-pseudofermion state equals the former one multiplied by the phase factor \( S_{\alpha\nu}(q_j) \) of Eq. (12). (Applying the scattering unitary \( \hat{S}_{\alpha\nu,\alpha'\nu'}^\phi \) operator onto its one-pseudofermion state of the many-pseudofermion "in" state also generates the corresponding one-pseudofermion state of the many-pseudofermion "out" state; The latter one-pseudofermion state equals the former one multiplied by the phase factor \( S_{\alpha\nu}(q_j) \) of Eq. (12).) It follows that the many-pseudofermion virtual states (and "in" states) are eigenstates of the above generator \( S \) (and \( S^\phi \)). The eigenvalue \( S_T \) of \( S \) belonging to a PS virtual state and the eigenvalue \( S_T^\phi \) of \( S^\phi \) belonging to a PS "in" state are given by,

\[
S_T = e^{iQ_T} = \prod_{\alpha\nu} \prod_{j=1}^{N_{\alpha\nu}} S_{\alpha\nu}(q_j); \quad Q_T = \sum_{\alpha\nu} \sum_{j=1}^{N_{\alpha\nu}} Q_{\alpha\nu}(q_j)
\]

\[
S_T^\phi = e^{iQ_T^\phi} = \prod_{\alpha\nu} \prod_{j=1}^{N_{\alpha\nu}} S_{\alpha\nu}^\phi(q_j); \quad Q_T^\phi = \sum_{\alpha\nu} \sum_{j=1}^{N_{\alpha\nu}^*} Q_{\alpha\nu}^\phi(q_j).
\]
The "out" state equals the virtual state multiplied by the phase factor $S_T$ and the "in" state multiplied by $S^\Phi_T$. Since the "out" state is by construction an energy eigenstate of the 1D Hubbard model, this result confirms that the corresponding virtual and "in" states are also energy eigenstates of the model. The general expressions (8) and (14) for the functionals $Q^\Phi_{\alpha\nu}(q_j)$ and $Q_{\alpha\nu}(q_j)$ define uniquely the eigenvalues $S^\Phi_T$ and $S_T$ of $\hat{S}^\Phi$ and $\hat{S}$ for any PS "in" state and virtual state, respectively. Since these many-pseudofermion states equal the "out" excited energy eigenstate except for a phase factor, in this paper we often associate both $S$ matrices $S_{\alpha\nu}(q_j)$ and $S^\Phi_{\alpha\nu}(q_j)$ of Eq. (12) indifferently with the corresponding excited energy eigenstate, yet they are eigenvalues of one-pseudofermion states of the virtual and "in" states, respectively.

When moving around the lattice ring the $\alpha\nu$ pseudofermion (or hole) departs from the point $x = 0$ and arrives to $x = L$, one finds that,

$$\lim_{x \to L} \tilde{q} x = q x + Q^0_{\alpha\nu} + Q^\Phi_{\alpha\nu}(q) = q x + Q_{\alpha\nu}(q),$$

where $q$ refers to the virtual state. For this asymptote coordinate choice, $Q_{\alpha\nu}(q)$ is the overall $\alpha\nu$ pseudofermion (or hole) phase shift whose value is defined only to within addition of an arbitrary multiple of $2\pi$. From analysis of Eqs. (8) and (14), it follows that $2\pi \Phi_{\alpha\nu',\alpha'\nu'}(q_{j1}, q_{j2})$ is an elementary two-pseudofermion phase shift. The studies of Refs. [18, 19] consider other asymptote coordinates usually used in standard quantum non-relativistic scattering theory, such that $x \in (-L/2, +L/2)$ and thus $\delta_{\alpha\nu}(q) = Q_{\alpha\nu}(q)/2$ is the overall $\alpha\nu$ pseudofermion or hole phase shift given only to within addition of an arbitrary multiple of $\pi$. Furthermore, $\pi \Phi_{\alpha\nu',\alpha'\nu'}(q_j, q_j')$ is an elementary two-pseudofermion phase shift. However, the choice of either definition is a matter of taste and the uniquely defined quantity is the $S$ matrix.

Finally, an important property of the pseudofermion scattering theory introduced in Refs. [18, 19] is that the $\pm 1/2$ Yang holons and $\pm 1/2$ HL spinons are scatter-less objects. Indeed, the form of the scattering part of the overall phase shift (14), Eq. (9), reveals that the value of such a phase-shift functional is independent of the changes in the occupation numbers of the $\pm 1/2$ Yang holons and $\pm 1/2$ HL spinons. Thus, these objects are not scattering centers. Moreover, they are not scatterers, once their wave functions do not acquire any phase factor under the "in"-state - "out"-state transitions.

### B. PHASE SHIFTS IN THE REDUCED SUBSPACE

Within the pseudofermion description, the $m = 0$ and $n = 1$ initial ground state is such that the $c0$ and $s1$ bands are full and thus the Fermi momentum values given in Eq. (5) coincide with the corresponding limiting values provided in the same equation and are such that $q^0_{\alpha\nu,c0} = q^0_{\alpha\nu,s1} = \pi$ and $q^0_{\alpha\nu,s1} = q^0_{\alpha\nu,c0} = \pi/2$. The reduced subspace considered in the studies of Refs. [22, 23, 24] is spanned by twelve types of excited energy eigenstates of that ground state. The excited states belonging to each of these types are characterized by fixed values for the numbers of holes in the $c0$ and $s1$ bands, $\eta$ spin $\eta = S_0 = \Delta S_0, \eta$-spin projection $\eta_2 = S_2^\phi = \Delta S_2^\phi$, spin $S = S_0 = \Delta S_0$, and spin projection $S_2 = S_2 = \Delta S_2$. Here $\Delta S_0, \Delta S_2, \Delta S_0^\phi$, and $\Delta S_2^\phi$ are the deviations relative to the values of the $m = 0$ and $n = 1$ initial ground state. For excited states of that state such deviations equal the corresponding values of $S_0, S_0^\phi$, $S_2$, and $S_2^\phi$, respectively. If one specifies the two bare-momentum values of the created holes, each of such classes of states corresponds to a uniquely defined excited energy eigenstate. Thus, each class of states is generated from one of these energy eigenstates by considering all possible bare-momentum values of the two created pseudofermion holes.

The values of the numbers which characterize each class of excited states are provided in Table I. In order to give information about the pseudofermions, Yang holons, and HL spinons created or annihilated under the ground-state - excited-state transitions, we also provide in that table the values for the deviations $\Delta N$ in the spin-projection $\sigma$ electronic numbers and $\Delta M_{\sigma \pm 1/2}$ of $\pm 1/2$ holons ($\alpha = c$) and $\pm 1/2$ spinons ($\alpha = c$) [10]. (In CPHS ensemble space, CPHS refers to $c0$ pseudofermion, holon, and spinon.) In Table II we provide the values of the corresponding deviations $\Delta N_\sigma$ in the spin-projection $\sigma$ electronic numbers and $\Delta M_{\sigma \pm 1/2}$ in the $\pm 1/2$ holon ($\alpha = c$) and $\pm 1/2$ spinon ($\alpha = s$) numbers of the pseudofermion representation of Refs. [29, 31] for each class of excited states of Table I. Moreover, in Table II we also provide the values of the scatter-less phase shifts $Q^0_{\alpha\nu,c0}$ and $Q^\Phi_{\alpha\nu,s1}$ given in Eq. (14) of Appendix A for these states. We note that the numbers of spinons and holons of spinons and the alternative spinon-holon representation of Refs. [22, 23, 24] equal the numbers $N^h_{\alpha\nu,s1} = \Delta N^h_{\alpha\nu,s1}$ of spin holes and $N^h_{\alpha\nu,c0} = \Delta N^h_{\alpha\nu,c0}$ of charge holes, respectively, given in Table I.

Within the pseudofermion description, two out of the twelve types of excited states of Table I have one $\alpha\nu \neq c0, s1$ pseudofermion: the $\eta$-spin singlet excited states and spin singlet excited states have one $c1$ pseudofermion and one $s2$
pseudofermion, respectively. While for initial ground states with densities in the ranges $0 < n < 1$ and $0 < m < n$ the $\alpha\nu \neq c\delta$, $s1$ pseudofermions are scatterers, it was found in Ref. [19] that for excited energy eigenstates of a $n = 1$ and $m = 0$ initial ground state with a single $\alpha\nu \neq c\delta$ pseudofermion (and $s\nu \neq s1$ pseudofermion), such a quantum object has bare momentum $q = 0$, canonical momentum $\bar{q} = q = 0$, and is invariant under the electron - rotated-electron unitary transformation. Since $\bar{q} = q = 0$, such a $\alpha\nu \neq c\delta$ pseudofermion (and $s\nu \neq s1$ pseudofermion) is not a scatterer. This implies that $Q_{c1}(0) = 0$ and $Q_{s2}(0) = 0$ for the overall phase shift given in Eq. (11) corresponding to the $c1$ pseudofermion and $s2$ pseudofermion, respectively, created under the transition from the ground state to the $c\eta$-spin singlet and spin singlet excited state, respectively. It follows that for the $n = 1$ (and $m = 0$) initial ground state there is no one-pseudofermion scattering state for the $c1$ pseudofermion (and $s2$ pseudofermion). Thus, within the pseudofermion scattering theory, for all the reduced-subspace excited energy eigenstates of Table I the only quantum objects that are both scatterers and scattering centers are the $c\delta$ pseudofermion holes and/or the $s1$ pseudofermion holes created under the ground-state - excited-state transitions.

Here we calculate all the $c\delta$ and $s1$ pseudofermion-hole overall phase shifts associated with the types of excited states of Table I. Interestingly, we show that for such excited states the overall pseudofermion-hole phase shifts $Q_{c0}(q)$ and $Q_{s1}(q)$ defined by the general overall phase-shift expression (11) have the same values as the holon and spinon phase shifts, respectively, considered in Refs. [22-24]. (For the phase shift $Q_{c0}(q)$ this is true except for a constant term, as further discussed below.)

Let us show that the phase shifts provided in Eqs. (5.19)-(5.21) of Ref. [24] correspond indeed to particular cases of the overall pseudofermion-hole phase shift functionals $Q_{c0}(q)$ and $Q_{s1}(q)$ defined by Eq. (11). (We recall that such phase shifts refer to a pseudofermion hole when the corresponding bare-momentum value $q$ is empty for the excited state.) In Appendix A we provide the bare-momentum distribution-function deviations of the twelve classes of excited states of Tables I and II. Use of Eqs. (A2)-(A6) of that Appendix in Eqs. (9) and (11) for the overall phase shift leads to,

$$Q_{c0}(q) = -\pi \left[ 2 \sum_{l=1}^{2} \Phi_{c0,c0}(q, q_l) - \Phi_{c0,c0}(q, \pi) + \Phi_{c0,c0}(q, -\pi) + \Phi_{c0,s1}(q, \pi/2) + \Phi_{c0,s1}(q, -\pi/2) \right], \quad (16)$$

for the three classes of $\eta$-spin triplet states,

$$Q_{c0}(q) = -\pi \left[ 2 \sum_{l=1}^{2} \Phi_{c0,c0}(q, q_l) + \Phi_{c0,s1}(q, \pi/2) + \Phi_{c0,s1}(q, -\pi/2) - 2\Phi_{c0,c1}(q, 0) \right], \quad (17)$$

for the $\eta$-spin singlet states,

$$Q_{s1}(q) = -\pi \left[ 2 \sum_{l=1}^{2} \Phi_{s1,s1}(q, q_l') - \Phi_{s1,c0}(q, \pi) + \Phi_{s1,c0}(q, -\pi) - \Phi_{c0,s1}(q, \pi/2) - \Phi_{c0,s1}(q, -\pi/2) \right], \quad (18)$$

\begin{table}[h]
\begin{tabular}{|c|c|c|c|c|c|c|c|c|c|c|c|c|c|}
\hline
Excited state & Charge holes & Spin holes & $\eta$ & $\eta_s$ & $S$ & $S_N$ & $\Delta N_{c0}$ & $\Delta N_{s1}$ & $N_{c0}$ & $N_{s1}$ & $L_{c,-1/2}$ & $L_{c,+1/2}$ & $L_{s,-1/2}$ & $L_{s,+1/2}$ \\
\hline
$\eta$-spin triplet & 2 & 0 & 1 & 1 & 0 & 0 & -2 & -1 & 0 & 0 & 2 & 0 & 0 & 0 \\
\hline
$\eta$-spin triplet & 2 & 0 & 1 & 0 & 0 & 0 & -2 & -1 & 0 & 1 & 1 & 0 & 0 & 0 \\
\hline
$\eta$-spin triplet & 2 & 0 & 1 & -1 & 0 & 0 & -2 & -1 & 0 & 0 & 2 & 0 & 0 & 0 \\
\hline
$\eta$-spin singlet & 2 & 0 & 0 & 0 & 0 & 0 & -2 & -1 & 1 & 0 & 0 & 0 & 0 & 0 \\
\hline
spin triplet & 0 & 2 & 0 & 0 & 1 & 1 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 2 \\
\hline
spin triplet & 0 & 2 & 0 & 0 & 1 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 2 \\
\hline
spin singlet & 0 & 2 & 0 & 0 & 1 & -1 & 0 & -1 & 0 & 0 & 0 & 0 & 2 & 0 \\
\hline
doublet & 1 & 1 & 1/2 & 1/2 & 1/2 & 1/2 & -1 & -1 & 0 & 0 & 0 & 1 & 0 & 1 \\
\hline
doublet & 1 & 1 & 1/2 & -1/2 & 1/2 & 1/2 & -1 & -1 & 0 & 0 & 0 & 1 & 0 & 1 \\
\hline
doublet & 1 & 1 & 1/2 & 1/2 & 1/2 & -1/2 & -1 & -1 & 0 & 0 & 0 & 1 & 0 & 1 \\
\hline
doublet & 1 & 1 & 1/2 & -1/2 & 1/2 & -1/2 & -1 & -1 & 0 & 0 & 0 & 1 & 0 & 1 \\
\hline
\end{tabular}
\end{table}
for the three classes of spin triplet states,
\[ Q_{s1}(q) = -\pi \left[ 2 \sum_{l=1}^{2} \Phi_{s1, s1}(q, q') - \Phi_{s1, c0}(q, \pi) + \Phi_{s1, c0}(q, -\pi) - 2 \Phi_{s1, s2}(q, 0) \right], \]  
(19)
for the spin singlet states and,
\[ Q_{c0}(q) = -\pi \left[ 2 \Phi_{c0, c0}(q, q') + 2 \Phi_{c0, s1}(q, q') \right]; \quad Q_{s1}(q) = -\pi \left[ 2 \Phi_{s1, c0}(q, q') + 2 \Phi_{s1, s1}(q, q') \right], \]  
(20)
for the four classes of doublet states.

By taking the limits \( m \to 0 \) and \( n \to 1 \) in the above expressions (16)- (20) for the phase shifts \( Q_{c0}(q) \) and \( Q_{s1}(q) \) at \( q = q_1 \) and \( q = q'_1 \), respectively, we find,
\[ Q_{c0}(q_1) = 2\pi B \left( \frac{\sin k_1 - \sin k_2}{u} \right) = \delta_{CT} - \pi, \]  
(21)
for the \( \eta \)-spin triplet states,
\[ Q_{c0}(q_1) = -2 \arctan \left( \frac{\sin k_1 - \sin k_2}{2u} \right) + 2\pi B \left( \frac{\sin k_1 - \sin k_2}{u} \right) = \delta_{CS} - \pi, \]  
(22)
for the \( \eta \)-spin singlet states,
\[ Q_{s1}(q'_1) = -2\pi B \left( \frac{\Lambda'_1 - \Lambda'_2}{u} \right) = \delta_{ST}, \]  
(23)
for the spin triplet states,
\[ Q_{c0}(q'_1) = 2 \arctan \left( \frac{\Lambda'_1 - \Lambda'_2}{2u} \right) - 2\pi B \left( \frac{\Lambda'_1 - \Lambda'_2}{u} \right) = \delta_{SS}, \]  
(24)
for the spin singlet states and,
\[ Q_{c0}(q_1) = \arctan \left( \frac{\sin \left( \frac{\pi}{2} \left[ \frac{\sin k_1 - \Lambda'_1}{u} \right] \right)}{2}\right) = \delta_{\eta S} - \pi; \quad Q_{s1}(q'_1) = \arctan \left( \frac{\pi}{2} \left[ \frac{\Lambda'_1 - \sin k_1}{u} \right] \right) = \delta_{\eta S}, \]  
(25)
for the doublet states. To derive these \( m \to 0 \) and \( n \to 1 \) phase-shift expressions we used Eqs. (A7) - (A11) of Appendix A. For the phase shift of the \( \eta \)-spin singlet (and spin singlet) states we also used the two-pseudofermion phase-shift expression given in Eq. (13) of that Appendix. In the above overall phase-shift expressions, \( k_1 = k^0(q_1), k_2 = k^0(q_2), \Lambda^0_1(q) = \sin k^0(q), \Lambda_1 = \Lambda^0_1(q'_1), \Lambda_2 = \Lambda^0_1(q'_2) \), the rapidity functions \( k^0(q) \) and \( \Lambda^0_1(q) \) are the inverse of the functions defined by the first and second equations of Eq. (A.1) of Ref. 15, respectively, with \( \nu = 1 \) in the second equation, the function \( B(r) \) is defined in Eq. (A12) of Appendix A, and \( u = \frac{U}{4t} \).

By inspection of the above phase-shift expressions one indeed confirms that \( \pi + Q_{c0}(q_1) \) with \( Q_{c0}(q_1) \) provided in Eqs. (21), (22), and (23) equals the phase shifts \( \delta_{CT}, \delta_{CS}, \) and \( \delta_{\eta S}, \) respectively, given in Ref. 24. The two former phase shifts are provided in Eq. (5.19) and the latter in Eq. (5.21) of that reference. Moreover, the phase shift \( Q_{s1}(q'_1) \) provided in Eqs. (23), (24), and (25) equals the phase shifts \( \delta_{ST}, \delta_{SS}, \) and \( \delta_{\eta S}, \) respectively, given in the same reference. In this case the two former phase shifts are provided in Eq. (5.20) and the latter in Eq. (5.21) of Ref. 24. For the phase shifts of the doublet excited states the confirmation of the above equalities also involves that \( \arctan(\sin(\pi x)) = 2 \arctan(\exp(\pi x)) - \pi/2 \) for the branch such that these functions vary between \(-\pi/2 \) and \(+\pi/2 \).

Note that the phase shifts \( \delta_{CT} \) and \( \delta_{CS} \) given in Eq. (5.19) and \( \delta_{\eta S} \) in Eq. (5.21) of Ref. 24 read \( \pi + Q_{c0}(q_1) \), whereas according to the phase-shift definition of Eq. (15) the corresponding \( c0 \) pseudofermion-hole phase shifts are given by \( Q_{c0}(q_1) \). The studies of Ref. 24 used the method of Ref. 32 to evaluate the above phase shifts. That method provides the phase shifts up to an overall constant term. In contrast, the method of Refs. 18, 19 provides the full corresponding pseudofermion-hole phase shift value. In reference 24 the term \( \pi \) was added so that in the limit \( U \to \infty \) the phase factor \( \exp (i\delta_{CT}) \) reads \( \exp (i\delta_{CT}) = 1 \). However, the \( c0 \) pseudofermion and hole phase shifts \( Q_{c0}(q) \) of Eq. (15) fully agree with the corresponding \( U \to \infty \) shifts used in the exact one-electron spectral-function studies of Ref. 33. For the scattering properties alone the constant extra term \( \pi \) of the phase shifts \( \delta_{CT}, \delta_{CS}, \) and \( \delta_{\eta S} \) calculated in Ref. 24 is unimportant. In contrast, the use of the correct overall pseudofermion-hole phase shift \( Q_{c0}(q) \) defined as in Eq. (15) is required in the applications of the scattering theory to the study of the finite-energy spectral properties 2, 13, 16, 33.
A first important result for the clarification of the relation between the two representations is that in the reduced subspace the holon-scatterer and spinon-scatterer phase shifts of the conventional spinon-holon representation of Refs. 22, 23, 24 equal the $c_0$ pseudofermion-hole and $s_1$ pseudofermion-hole phase shifts of the pseudofermion representation of Refs. 18, 19, respectively. (Except for $\pi$ for the holon scatterers.) Moreover, in this section we have shown that the phase shifts of the conventional spinon-holon representation are particular cases of the $c_0$ and $s_1$ pseudofermion overall phase-shift functionals $Q_{\alpha\nu}(q)$ defined by Eq. (11). The pseudofermion scattering theory refers to any initial ground state for densities in the ranges $0 \leq n \leq 1$ and $0 \leq m \leq n$, whereas the spinon-holon scattering theory corresponds to the $n = 1$ and $m = 0$ initial ground state only. Furthermore, while the pseudofermion scattering theory is associated with a larger excitation subspace, which coincides with the PS, the phase shifts studied in Refs. 22, 23, 24 correspond to a reduced subspace spanned by the types of excited states of Tables I and II.

### C. RELATION BETWEEN THE TWO CHOICES OF SCATTERING STATES AND CORRESPONDING S MATRICES IN THE REDUCED SUBSPACE

The above results enable us to relate the one-particle $S$ matrices of the two representations in the reduced subspace. Such an analysis provides useful information about the connection between the corresponding scattering states. For the pseudofermion representation the expression of the unitary $\hat{S}$ operator which generates the virtual-state - "out" - state transition factorizes as $\hat{S} = \prod_{\alpha\nu} \prod_{j=1}^{\eta_{\alpha\nu}} S_{\alpha\nu,q_j}$. Consistently, the excited energy eigenstates can be written as a direct product of one-pseudofermion states. It follows that application of the unitary $\hat{S}_{\alpha\nu,q_j}$ operator onto a many-pseudofermion virtual state gives that state multiplied by the $S$ matrix $S_{\alpha\nu,q_j}$ given in Eq. (12). Thus, one can consider that both the many-pseudofermion virtual state and its one-pseudofermion state corresponding to the $\alpha\nu$ branch and bare-momentum $q_j$ are eigenstates of $\hat{S}_{\alpha\nu,q_j}$ with the same eigenvalue $S_{\alpha\nu}(q_j)$.

We have shown in the previous subsection that in the reduced subspace spanned by the types of excited energy eigenstates of Tables I and II the holon (and spinon) phase shift of the conventional spinon-holon representation equals except for $\pi$ (and equals) the corresponding phase shift of the $c_0$ pseudofermion-hole scatterer (and $s_1$ pseudofermion-hole scatterer) corresponding to the same bare-momentum value $q_j = 2\pi/I_j^{10}$ (and $q_j = 2\pi/I_j^{11}$). This reveals that the $S$ matrix associated with the one-particle holon and spinon $S$ operator can also be obtained by application of the latter operator onto either the one-particle state or the corresponding many-particle state.

Both the holons (and spinons) of the spinon-holon representation and the $c_0$ pseudofermion holes (and $s_1$ pseudofermion holes) correspond to the unoccupied quantum numbers $I_j^{00}$ of the BA charge distribution of $k$'s excitations (of the unoccupied quantum numbers $I_j^{11}$ of the BA spin string excitations of length one). However, that the holons (and spinons) of the spinon-holon representation and the $c_0$ pseudofermion holes (and $s_1$ pseudofermion holes) refer to the same unoccupied BA quantum numbers $I_j^{00}$ (and $I_j^{11}$) does not imply that their one-particle states are the same. Indeed, the holon (and spinon) of momentum $q_j$ carries $\eta$-spin 1/2 (and spin 1/2), whereas the corresponding $c_0$ pseudofermion hole (and $s_1$ pseudofermion hole) of momentum $q_j$ is a $\eta$-spin-less and spin-less object (and is a spin-zero object), as further discussed in Sec. IV. Therefore, the relation of the one-pseudofermion scattering states to the holon or spinon one-particle scattering states of the conventional spinon-holon representation is a complex problem.

| Excited state | $\Delta N_\pi$ | $\Delta N_\eta$ | $\Delta M_{c, -1/2}$ | $\Delta M_{c, 1/2}$ | $\Delta M_{s, -1/2}$ | $\Delta M_{s, 1/2}$ | $Q_{\alpha\nu}^{00}$ | $Q_{\alpha\nu}^{11}$ |
|--------------|----------------|----------------|---------------------|---------------------|---------------------|---------------------|---------------------|---------------------|
| $\eta$-spin triplet | -1 | -1 | 0 | 2 | -1 | -1 | $\pm \pi$ | $\pm \pi$ |
| $\eta$-spin triplet | 0 | 0 | 1 | 1 | -1 | -1 | $\pm \pi$ | $\pm \pi$ |
| $\eta$-spin triplet | 1 | 1 | 2 | 0 | -1 | -1 | $\pm \pi$ | $\pm \pi$ |
| $\eta$-spin singlet | 0 | 0 | 1 | 1 | -1 | -1 | $\pm \pi$ | $\pm \pi$ |
| spin triplet | 1 | -1 | 0 | 0 | -1 | 1 | $\pm \pi$ | $\pm \pi$ |
| spin triplet | 0 | 0 | 0 | 0 | 0 | 0 | $\pm \pi$ | $\pm \pi$ |
| spin triplet | -1 | 1 | 0 | 0 | 0 | 1 | $\mp \pi$ | $\pm \pi$ |
| spin singlet | 0 | 0 | 0 | 0 | 0 | 0 | $\pm \pi$ | $\pm \pi$ |
| doublet | 0 | 1 | 1 | 0 | 0 | -1 | $\pm \pi$ | 0 |
| doublet | -1 | 0 | 0 | 1 | 0 | -1 | $\pm \pi$ | 0 |
| doublet | 1 | 0 | 1 | 0 | -1 | 0 | $\pm \pi$ | 0 |
| doublet | 0 | -1 | 0 | 1 | -1 | 0 | $\pm \pi$ | 0 |

TABLE II: The values of the spin-projection $\sigma$ electronic number deviations $\Delta N_\pi, \pm 1/2$ holon $(\alpha = c)$ and $\pm 1/2$ spinon $(\alpha = s)$ number deviations $\Delta M_{c,s, \pm 1/2}$ for the pseudofermion representation of Refs. 22, 23, and scatter-less phase shifts $Q_{\alpha\nu}^{00}$ and $Q_{\alpha\nu}^{11}$ of Eq. (11) of Appendix A for each class of excited states of Table I.
Fortunately, useful information about the relation between the one-particle scattering states of both representations can be obtained by studying the connection between the set of corresponding many-particle excited states of the two representations with the precisely the same occupancy configurations of the BA $I^{0}_j$ and $I^{1}_j$ quantum numbers. For each of the two alternative representations we replace the one-particle state under consideration by a suitable many-particle excited state with the same eigenvalue for the one-particle $S$ operator and thus with the same value for the one-particle $S$ matrix. The relation between the many-particles states of both representations is easier to achieve and provides important information about the corresponding one-particle scattering states.

Within the spinon-holon representation of Refs. [23, 24], the scatters and scattering centers are the $\pm 1/2$ spinons and $\pm 1/2$ holons created under the ground-state - excited state transitions. For the reduced subspace considered in these references, this leads to a spinon-spinon $4 \times 4$ $S$ matrix, a holon-holon $4 \times 4$ $S$ matrix, and a related $16 \times 16$ $S$ matrix for the full scattering problem, as explained below. The holon-holon $4 \times 4$ $S$ matrix (and spinon-spinon $4 \times 4$ $S$ matrix) corresponds to the subspaces spanned by the four types of $\eta$-spin triplet and singlet excited energy eigenstates (and spin triplet and singlet excited states) considered in Tables I and II. In this case the two objects created under the ground-state - excited-state transitions are holons (and spinons) and thus it is unimportant which of them is chosen as scatterer and scattering center, since the phase shifts are the same. Thus, if one considers fixed momentum values for the two created objects the number of relevant one-particle scattering states equals that of excited energy eigenstates. In turn, for each of the above considered four types of doublet excited energy eigenstates, one must consider two one-particle scattering states. Indeed, as given in Table I, in this case one holon and one spinon are created under the ground-state - excited-state transitions and thus the one-particle scattering states where that holon and spinon is the scatterer are different: the holon and spinon scattering states are associated with different phase shifts which refer to the $c0$ and $s1$ phase shifts of Eq. (25), respectively. Therefore, while at fixed momentum values of the two created objects the reduced subspace is spanned by the twelve excited energy eigenstates considered in Table I, the $S$ matrix for the corresponding full scattering problem involves sixteen states and thus has dimension $16 \times 16$. However, for each pair of one-particle scattering states associated with the same doublet energy eigenstate one uses the latter state in the evaluation of the corresponding phase shifts which appear in the entries of that $S$ matrix. It is of the form,

$$ S = \begin{bmatrix} S_{SS} & 0 & 0 & 0 \\ 0 & S_{S\eta} & 0 & 0 \\ 0 & 0 & S_{\eta S} & 0 \\ 0 & 0 & 0 & S_{CC} \end{bmatrix}, \tag{26} $$

where $S_{S\eta}$ and $S_{\eta S}$ are $4 \times 4$ diagonal matrices corresponding to scattering events where the spinons and holons are the scatters and the holons and spinons the scattering centers, respectively. In turn, $S_{SS}$ and $S_{CC}$ are the above two $4 \times 4$ $S$ matrices associated with the spinon-spinon and holon-holon scattering, respectively. The latter two matrices are not diagonal. We denote the corresponding two sets of four states which correspond to the four one-particle scattering states by $|+1/2,+1/2; \alpha\rangle$, $|-1/2,-1/2; \alpha\rangle$, $|+1/2,-1/2; \alpha\rangle$, and $|-1/2,+1/2; \alpha\rangle$, where $\alpha = c$ and $\alpha = s$ refer to the holon-holon and spinon-spinon states, respectively. The two $\eta$-spin ($\alpha = c$) or spin ($\alpha = s$) projections $\pm 1/2$ labeling these states are those of the two involved holons or spinons, respectively. The $4 \times 4$ permutation matrix $P$ transforms these four states as,

$$ |+1/2,+1/2; \alpha\rangle \implies |+1/2,+1/2; \alpha\rangle; \quad |+1/2,-1/2; \alpha\rangle \implies |-1/2,+1/2; \alpha\rangle, \tag{27} $$

$$ |-1/2,+1/2; \alpha\rangle \implies |+1/2,-1/2; \alpha\rangle; \quad |-1/2,-1/2; \alpha\rangle \implies |-1/2,-1/2; \alpha\rangle; \quad \alpha = c, s. \tag{27} $$

The two above non-diagonal matrices $S_{SS}$ and $S_{CC}$ are then of the following form,

$$ S_{\beta\beta} = \frac{1}{2}(S_{\beta T} + S_{\beta S}) I + \frac{1}{2}(S_{\beta T} - S_{\beta S}) P; \quad \beta = C, S, \tag{28} $$

where $I$ is the $4 \times 4$ unity matrix,

$$ S_{\beta\tau} = (-1)^{y_{\beta}} e^{i\delta_{\beta\tau}}; \quad \beta = C, S; \quad \tau = T, S; \quad y_C = 1, \quad y_S = 0, \tag{29} $$

and $\delta_{\beta\tau}$ with $\beta = C, S$ and $\tau = T, S$ are the four phase shifts defined by Eqs. (21), (22), (23), and (24). In turn, the four diagonal entries of the above $4 \times 4$ diagonal matrices $S_{S\eta}$ and $S_{\eta S}$ are equal and given by,

$$ S_{\beta'\beta''} = (-1)^{y_{\beta''}} e^{i\delta_{\beta'\beta''}}; \quad \beta'\beta'' = S\eta, \eta S; \quad z_\eta = 1, \quad z_S = 0, \tag{30} $$

where $\delta_{\beta'\beta''}$ with $\beta'\beta'' = S\eta, \eta S$ are the two phase shifts defined in Eq. (25).

As discussed above, the pseudofermion-representation method for evaluation of phase shifts of Refs. [18, 19] leads to the general phase-shift functional expression defined by Eqs. (6) and (14). Such a method provides the full phase-shift
expressions. In contrast, the method of Ref. 33 used in the studies of Refs. 23, 24 provides the phase shifts (and corresponding $S$ matrices) of the reduced-subspace excited states except for an overall constant term (and an overall constant factor). This is behind a factor $-1$ appearing in the $S$ matrices given in Eqs. 29 and 30 for $\beta = C$ and $\beta' = \gamma$, respectively, relative to the corresponding $S$ matrices of Refs. 23, 24.

Within the pseudofermion representation of Refs. 18, 19, we denote the four excited energy eigenstates associated with the four one-particle scattering states of the alternative (and spinon-spinon) representation as follows, the four one-particle scattering states of the alternative (and spinon-spinon) representation as follows, $|\eta 0\rangle$ (and $|\eta 2; 0\rangle$) correspond to the four holon-holon excited states (and three spin triplet excited states) considered in Table I. Our analysis involves the phase shift of the $c_0$ (and $s_1$) pseudofermion-hole scatterer. Indeed, the two branch indices $c_0, c_0$ (and $s_1, s_1$) of these states refer to the $c_0$ (and $s_1$) pseudofermion-hole scatterer and $c_0$ (and $s_1$) pseudofermion-hole scattering center, respectively. In turn, $|c_0, c_1, 0\rangle$ (and $|s_1, s_1, 0\rangle)$ denotes the $\eta$-spin singlet excited state (and spin singlet excited state) whose three branch indices $c_0, c_0, c_1$ (and $s_1, s_1, s_2$) refer to the $c_0$ pseudofermion-hole scatterer, $c_0$ pseudofermion-hole scattering center, and $c_1$ pseudofermion scattering center (and $s_1$ pseudofermion-hole scatterer, $s_1$ pseudofermion-hole scattering center, and $s_2$ pseudofermion scattering center).

In contrast, the eight one-particle scattering states of Refs. 23, 24 associated with ground-state - excited-state transitions where one holon and one spinon are created correspond to only the four doublet excited energy eigenstates considered above. Moreover, in that case the four many-particle states of both representations associated with these eight one-particle scattering states are the same states. However, the absence of one-to-one correspondence between the other eight many-particle states associated with the eight one-particle scattering states involving objects of the same type (two spinons or two holons for the spinon-holon representation of Refs. 23, 24) and the corresponding eight excited energy eigenstates implies that the $16 \times 16$ $S$ matrix corresponding to the reduced-subspace scattering problem has a different form for the two representations. In the case of the pseudofermion representation of Refs. 18, 19, we find for the reduced subspace a diagonal $16 \times 16$ $S$ matrix which is related to the non-diagonal $S$ matrix given in Eq. 29 by a unitary transformation as follows,

$$\bar{S} = U^\dagger S U = \begin{bmatrix} \bar{S}_{SS} & 0 & 0 & 0 \\ 0 & \bar{S}_{S\eta} & 0 & 0 \\ 0 & 0 & \bar{S}_{\eta S} & 0 \\ 0 & 0 & 0 & \bar{S}_{\eta\eta} \end{bmatrix} ; \quad U = \begin{bmatrix} J & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} ; \quad J = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1/\sqrt{2} & -1/\sqrt{2} & 0 \\ 0 & 1/\sqrt{2} & 1/\sqrt{2} & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

(31)

Here the matrix $U$ is unitary. The three first diagonal entries (and the fourth diagonal entry) of the two $4 \times 4$ diagonal matrices $\bar{S}_{S\alpha}$ such that $\alpha = G$, $S$ of the above $\bar{S}$ expression equal the phase factor $\beta ST$ (and equals the phase factor $\beta ST$ given in Eq. 29). The four diagonal entries of the other two $4 \times 4$ diagonal matrices $\bar{S}_{\alpha\eta}$ such that $\beta' \beta'' = S_{\eta\eta}$ of the same expressions are equal and given in Eq. 30. For the general pseudofermion scattering theory the diagonal entries of the $16 \times 16$ diagonal matrix $\bar{S}$ provided in Eq. (31) are the sixteen $S$ matrices $S_{\alpha\eta}(q_j)$ of dimension one and of general form given in Eq. 12 corresponding to the $c_0$ and $s_1$ pseudofermion-hole scatterers of the reduced-subspace excited states considered here.

Use of the unitary matrix defined in Eq. 31 reveals that the above four holon-holon ($\alpha = c$) and four spinon-spinon ($\alpha = s$) states can be expressed in terms of the excited energy eigenstates which contain the one-pseudofermion scattering states of the alternative representation as follows,

$$| + 1/2, +1/2; \alpha \rangle = |\alpha \nu, \alpha \nu, -1\rangle ; \quad | + 1/2, -1/2; \alpha \rangle = \frac{1}{\sqrt{2}} \left[ |\alpha \nu, \alpha \nu, 0\rangle - |\alpha \nu, \alpha \nu, \alpha \nu\rangle \right] ,$$

$$| - 1/2, +1/2; \alpha \rangle = \frac{1}{\sqrt{2}} \left[ |\alpha \nu, \alpha \nu, 0\rangle + |\alpha \nu, \alpha \nu, \alpha \nu\rangle \right] ; \quad | - 1/2, -1/2; \alpha \rangle = |\alpha \nu, \alpha \nu, +1\rangle .$$

Here $\alpha \nu = c_0, s_1$ or $\alpha \nu' = c_1, s_2$, respectively. This confirms that the states $| + 1/2, -1/2; \alpha \rangle$ and $| - 1/2, +1/2; \alpha \rangle$ associated with the holon-holon and spinon-spinon one-particle scattering states of the conventional spinon-holon representation are not eigenstates of the $\eta$ spin ($\alpha = c$) or spin ($\alpha = s$).

IV. FAITHFUL CHARACTER AND SUITABILITY TO THE STUDY OF THE SPECTRAL PROPERTIES OF BOTH THEORIES IN THE PS

In this section we consider the extension of the scattering theory associated with the spinon-holon representation of Refs. 23, 24, 25 to the whole PS and show that similarly to the pseudofermion scattering theory it is faithful there.
Furthermore, we discuss the suitability of the two representations under consideration for applications to the study of the finite-energy spectral and dynamical properties.

A. FAITHFUL CHARACTER OF BOTH REPRESENTATIONS IN THE PS AND THE CHARGE AND SPIN CARRIED BY THE CORRESPONDING QUANTUM OBJECTS

The rotated-electron holon and spinon description introduced in Ref. 29 was shown in that reference to be a faithful representation for the whole Hilbert space. For the PS that the pseudofermion description refers to, by faithful representation we mean that for each subspace with fixed values of \( S_c \) of \( \eta \) spin, \( S \) of spin, \( M_c \) of the holon number, and \( M_s \) of the spinon number, the corresponding number of \( \eta \)-spin (and spin) irreducible representations equals the number of \( \nu \geq 1 \) composite \( cv \) pseudofermions and \(-1/2\) Yang holons (and \( \nu \geq 1 \) composite \( sv \) pseudofermions and \(-1/2\) HL spinons) occupancy configurations of the energy eigenstates that span such subspaces. The dimension of any PS subspace spanned by all energy eigenstates with fixed values of \( S_c, S, M_c, \) and \( M_s \) is given by

\[
\left( \frac{N_\alpha}{N_{\alpha 0}} \right) \times \mathcal{N}(S_c, M_c) \times \mathcal{N}(S_s, M_s).
\]

Here \( \mathcal{N}(S_c, M_c) \) and \( \mathcal{N}(S_s, M_s) \) is the number of states with fixed \( \eta \)-spin value \( S_c \) and spin value \( S_s \), respectively, representative of a collection of a number \( M_c \) of \( \eta \)-spin 1/2 holons and \( M_s \) of spin 1/2 spinons, respectively. The faithful character of this representation follows from the equality of the following two numbers: The number given in Eq. (47) of Ref. 29 of \( \eta \)-spin (\( \alpha = c \)) and spin (\( \alpha = s \)) irreducible representation states of \( M_c \) \( \eta \)-spin 1/2 holons and \( M_s \) spin 1/2 spinons, arranged within all possible configurations with fixed \( \eta \)-spin value \( S_c \) and spin value \( S_s \), respectively, and the number provided in (51) of that reference. The latter is the product of the number discrete bare-momentum \( av \) pseudofermion occupancy configurations such that the number of \( 2\nu \)-holon composite \( cv \) pseudofermions \( (\alpha = c) \) or \( 2\nu \)-spinon composite \( sv \) pseudofermions \( (\alpha = s) \) obey the sum rule \( \sum_{\nu=1}^{\infty} \nu N_{av} = [M_\alpha/2 - S_s] \) by the number of possible occupancies of the \(-1/2 \) and \(+1/2 \) Yang holons \( (\alpha = c) \) and \(-1/2 \) and \(+1/2 \) HL spinons \( (\alpha = s) \) such that \( L_\alpha = [L_{\alpha,+1/2} + L_{\alpha,-1/2}] = 2S_s \). In reference 29 it is shown that this equality occurs for all the above subspaces with fixed values for \( S_c, S_s, M_c, \) and \( M_s \). For the rotated-electron holon and spinon description of that reference the \( \eta \)-spin \( SU(2) \) irreducible representations correspond to the BA charge string excitations of length \( \nu = 1, 2, 3, \ldots \) and \( \pm 1/2 \) Yang holon occupancy configurations. Moreover, the number \( \left( \frac{N_\alpha}{N_{\alpha 0}} \right) \) of \( c0 \) pseudofermion and hole occupancy configurations appearing in Eq. 43 does not count \( \eta \)-spin \( SU(2) \) irreducible representations. This implies that within the rotated-electron holon and spinon definition of Ref. 29 the occupancy configurations of the \( c0 \) pseudofermion and holes of states belonging to the PS are independent of the \( \eta \)-spin degrees of freedom and thus are not related to the \( \eta \)-spin 1/2 holons. Moreover, note that according to Eq. (51) of Ref. 29 with \( \alpha = s \) the number of occupancy configurations \( \left( \frac{N_{s+1}}{N_{s+1 0}} \right) \) of the \( s+1 \) pseudofermions and holes (holes of the length-one spin string excitation spectrum) contribute to the number of spin singlet representation states with fixed \( S_s \leq M_s/2 \) value which according to the spin summation rules one can generate from \( M_s \) spin 1/2 spinons. This is consistent with the spin singlet character of the \( N_{s+1} \) two-spinon composite \( s+1 \) pseudofermions and \( N_{s+1}^h \) \( s+1 \) pseudofermion holes.

Let us next consider the spinon and holon definition of the conventional spinon-holon representation of Refs. 22, 24, 24. For the reduced subspace considered in the previous section, the spin 1/2 spinons are identified with the holes of the length-one BA spin string excitation spectrum. Moreover, the holes of the BA distribution of \( k \)'s excitation spectrum are identified with single \( \eta \)-spin 1/2 holons. In order to confirm the faithful character of the spinon-holon representation of Refs. 22, 24, 24 and search whether it is suitable for the description of the finite-energy spectral and dynamical properties of the metallic phase, it is convenient to extend it to the whole PS and to initial ground states corresponding to densities in the ranges \( 0 < n < 1 \) and \( 0 < m < n \). In the remaining of this paper we call it extended spinon-hole representation or theory.

The extended spinon-hole representation assumes that the \( N_{ch}^h \) holes in the BA distribution of \( k \)'s excitation spectrum are \( \eta \)-spin 1/2 holons and the \( N_{ch}^h \) holes in the length-one BA spin string excitation spectrum are spin 1/2 spinons. Thus, for electronic densities \( n < 1 \) and spin densities \( m > 0 \) the initial ground state itself has a finite number of holons and spinons. Each ground-state - excited-state transition leads to new values \( N_{ch0}^h + \Delta N_{ch}^h + N_{ch1}^h + \Delta N_{ch1}^h \). For the PS the deviations \( \Delta N_{ch0}^h \) and \( \Delta N_{ch1}^h \) refer to a finite number of created holons and spinons, respectively. The excited states considered in Sec. III and in Refs. 22, 24 correspond to a particular case of this extended spinon-hole theory where \( N_{ch0}^h = N_{ch1}^h = 0 \) for the initial ground state and \( \Delta N_{ch0}^h + \Delta N_{ch1}^h = 2 \) for the excited states. Let us denote the number of holons and spinons of such an extended theory by \( M_c \equiv N_{ch0}^h \) and \( M_s \equiv N_{ch1}^h \), respectively. The relation between the numbers of holons and spinons of both representations is such that

\[
M_c = M_{c,+1/2} + M_{c,-1/2} = M_c; \quad M_s = M_{s,+1/2} + M_{s,-1/2} = M_s - 2 \sum_{\nu=1}^{\infty} N_{av}.
\]
and thus $M_s < M_s$. Here $M_{\alpha, \pm 1/2}$ denotes the number of $\eta$-spin-projection $\pm 1/2$ holons ($\alpha = e$) and spin-projection $\pm 1/2$ spinons ($\alpha = s$). As for the other representation, we call these objects $\pm 1/2$ holons and $\pm 1/2$ spinons, respectively. Since the spinon-holon representation of Refs. [22, 23, 24] corresponds to one-particle scattering states which are part of eigenstates of the $\eta$-spin and spin algebras, the above numbers $M_{\alpha, \pm 1/2}$ are related to the eigenvalues of these generators as follows,

$$-2S^2_\alpha = M_{\alpha, +1/2} - M_{\alpha, -1/2}; \quad \alpha = c, s. \quad (35)$$

Within the extended spinon-holon scattering theory the $\pm 1/2$ spinons and $\pm 1/2$ holons are the scatterers and scattering centers. Thus, it follows from the finite spin and $\eta$-spin value of such scatterers and scattering centers that some of the corresponding one-particle scattering states do not correspond to eigenstates of the total spin and $\eta$-spin, as confirmed in the previous section for states belonging to the reduced subspace. Moreover, we find below that, in contrast to the corresponding one-pseudofermion scattering states, for initial ground states with densities $n < 1$ and/or $m > 0$ some of the one-particle scattering states of the extended spinon-holon theory do not correspond to energy and momentum eigenstates.

By combining Eq. (35) with the relations given in Eq. (34) we find that,

$$M_{c, \pm 1/2} = M_{c, \pm 1/2}; \quad M_{s, \pm 1/2} = M_{s, \pm 1/2} - \sum_{\nu=1}^{\infty} N_{s\nu}. \quad (36)$$

However, the holon number equality $M_{c, \pm 1/2} = M_{c, \pm 1/2}$ does not imply that the $\pm 1/2$ holons of the extended spinon-holon representation are the same quantum objects as those of the pseudofermion representation, as confirmed below. Indeed, the holons of both representations have different expressions in terms of rotated electrons and thus transform differently under the electron - rotated-electron unitary transformation and carry a different elementary charge. Furthermore, in contrast to the holons of the pseudofermion representation, those of the extended spinon-holon representation have a momentum-dependent energy dispersion.

Let us confirm that the extended spinon-holon representation is also faithful in the PS. The dimension of a PS subspace spanned by all energy eigenstates with fixed values of $S_c$, $S_s$, $M_c$, and $M_s$ as given in Eq. (34) reads,

$$\mathcal{N}(S_c, M_c) = \frac{N_a}{M_a} \times \frac{N_s}{M_s} \times \mathcal{N}(S_c, M_c) \times \mathcal{N}(S_s, M_s). \quad (37)$$

Here $\mathcal{N}(S_c, M_c)$ and $\mathcal{N}(S_s, M_s)$ is the number of states with fixed $\eta$-spin value $S_c$ and spin value $S_s$, respectively, representative of a collection of a number $M_c$ of $\eta$-spin $1/2$ holons and $M_s$ of spin $1/2$ spinons, respectively. We emphasize that the PS subspaces with fixed values for $S_c$, $S_s$, $M_c$, and $M_s$ are smaller than those with fixed values for $S_c$, $S_s$, $M_c$, and $M_s$ as confirmed below. The faithful character of the alternative extended spinon-holon representation requires that the numbers $S_c$, $S_s$, $M_c$, and $M_s$ must obey the following equality,

$$\mathcal{N}(S_c, M_a) = (2S_a + 1) \left\{ \left( \frac{M_a}{M_a/2 - S_a} \right) - \left( \frac{M_a}{M_a/2 - S_a} - 1 \right) \right\} = (2S_a + 1) \sum_{\{N_{a\nu}\}} \prod_{\nu'=1+x_a}^{\infty} \left( \frac{N_{a\nu'} + N_{h\nu'}}{N_{a\nu'}} \right), \quad (38)$$

where $\alpha = c, s$, the sum and product $\sum_{\{N_{a\nu}\}} \prod_{\nu'=1}^{\infty} (\nu' - x_a) N_{a\nu'} = [M_a/2 - S_a]$ is fix, $x_c = 0$, and $x_s = 1$. The factor $\left( \frac{M_a}{M_a/2 - S_a} - \left( \frac{M_a}{M_a/2 - S_a} - 1 \right) \right)$ in this equation is the number of $\eta$-spin ($\alpha = c$) and spin ($\alpha = s$) singlet representation states with fixed $S_a \leq M_a/2$ value which according to the $\eta$-spin and spin summation rules one can generate from $M_a$ quantum objects of $\eta$ spin $1/2$ and spin $1/2$, respectively. By multiplying this number by the number $(2S_a + 1)$ of states in each $SU(2)$ tower, one reaches the number of $\eta$-spin ($\alpha = c$) and spin ($\alpha = s$) irreducible representation states of $M_a$ $\eta$-spin $1/2$ holons and $M_a$ spin $1/2$ spinons, arranged within all possible configurations with fixed $\eta$-spin value $S_c$ and spin value $S_s$, respectively. In turn, the quantity $\sum_{\{N_{a\nu}\}} \prod_{\nu'=1}^{\infty} \left( \frac{N_{a\nu'} + N_{h\nu'}}{N_{a\nu'}} \right)$ on the right-hand side of Eq. (38) gives the number of occupancy configurations of the BA quantum numbers such that the sum rule $\sum_{\nu'=1+x_a}^{\infty} (\nu' - x_a) N_{a\nu'} = [M_a/2 - S_a]$ is obeyed. Furthermore, $(2S_a + 1)$ refers to the tower of states outside the BA solution. The point is that the equality (38) is indeed valid for all PS subspaces with fixed values for $S_c$, $S_s$, $M_c$, and $M_s$. Thus, the spinon-holon representation is faithful both for the PS and the reduced subspace spanned by the types of excited states of Tables I of Sec. III.

For each of the subspaces with fixed values of $S_c$, $S_s$, $M_c$, and $M_s$ associated with the c0 pseudofermion, holon, and spinon representation of Refs. [22, 23, 24], the subspace dimension of Eq. (34) is a product of three numbers. Two of these numbers are nothing but the value given in Eq. (47) of Ref. [22] of different states with the same value of $S_c$ that, following the counting rules of $\eta$-spin and spin summation, one can generate from $M_a$ $\eta$-spin $1/2$ holons.
(\(\alpha = c\)) and spin 1/2 spinons (\(\alpha = s\)). These two values are uniquely defined by the fixed values of the total \(\eta\) spin and spin of the subspace and by the fixed numbers of \(\eta\) spin 1/2 holons and spin 1/2 spinons in that subspace. The third number corresponds to the \(c\) pseudofermion excitations. This is the number of states with the same value of \(M\) and \(s\) spinon-holon states with fixed \(S\) values that, following the counting rules of \(\eta\)-spin and spin summation, one can generate from \(M\), \(s\) spin 1/2 holons (\(\alpha = c\)) and spin 1/2 spinons (\(\alpha = s\)). These two values are uniquely defined by the fixed values of the total \(\eta\) spin and spin of the subspace and by the fixed numbers of \(\eta\) spin 1/2 holons and spin 1/2 spinons in that subspace. The other two factors refer to the different choices of momentum occupancy configurations of the \(M\), \(s\) and \(M\) spinons, respectively. (Such configurations correspond to the BA distribution of \(k\)'s for the holons and BA spin string excitations of length one for the spinons.) Indeed, in the extended spinon-holon representation the spinons and holons have momentum-dependent energy dispersions.

The faithful character of the extended spinon-holon representation is closely related to the faithful character of the pseudofermion representation. As a matter of fact, the number given in Eq. (47) of Ref. 24 of spin singlet representation states with fixed \(S\) and \(M\) values which according to the spin summation rules one can generate from \(M\), \(s\) spin 1/2 spinons of that reference can be expressed as the following summation over the numbers of spin singlet representation states with fixed \(S\) value but different numbers \(M\) of spin 1/2 spinons of the alternative extended spinon-holon representation,

\[
\frac{M_s}{M_s/2 - S_s} - \frac{M_s}{M_s/2 - S_s - 1} = \sum_{\{M_s\}} \frac{N_s}{M_s} \times \frac{M_s}{M_s/2 - S_s} - \frac{M_s}{M_s/2 - S_s - 1}
\]

Here \(M_s\) and \(S_s\) are fixed and for each allowed value of \(M_s\), there is one and only one value of \(N_s\) such that \(M_s = 2S_s + 2\sum_{v'=2}^{\infty} (v' - 1) N_{sv'}\) and \(N_s = [M_s/2 - S_s] - \sum_{v=2}^{\infty} v' N_{sv'}\), respectively. Thus, the summation on the right-hand side of Eq. (39) is over the dimensions of all subspaces with fixed values for \(S\), \(M\), \(s\) and \(M\) that are contained in a single subspace with fixed values of \(S\), \(M\), \(s\) and \(M\).

An interesting point is the following. For the extended spinon-holon representation whose number reads \(\left(\frac{N_s}{M_s}\right)\) do not correspond to irreducible representations of the spin \(SU(2)\) algebra, but instead refer to the momentum occupancy configurations of the \(M\) spinons over the available \(N_{s}\) discrete spin-rapidity momentum values, as confirmed by Eqs. (37) and (38). In contrast, for the pseudofermion representation the factor \(\left(\frac{N_s}{M_s}\right)\) contributes to the number of irreducible representations of the spin \(SU(2)\) algebra associated with the \(M\) spinons of spin 1/2. Moreover, while for the former representation \(\left(\frac{N_s}{M_s}\right)\) gives the number of momentum occupancy configurations of the \(M\) holons over the available \(N_s\) discrete distribution of \(k\)'s values, for the latter description \(\left(\frac{N_s}{M_s}\right)\) is the number of momentum occupancy configurations of the \(N_{s}\) \(c\) pseudofermions over the available \(N_s\) discrete bare-momentum values. In contrast to the holons of the extended spinon-holon representation, the \(c\) pseudofermions and holes have no \(\eta\)-spin degrees of freedom 2455. On the other hand, for the \(\alpha\) \(c\) \(\neq c\), \(s\) excitations the number of occupancy configurations \(\left(\frac{N_s}{N_{c0}}\right)\) contributes to the numbers of irreducible representations of the \(\eta\)-spin \(\alpha\) \(c\) \(\neq c\) and spin \(\alpha\) \(\neq\) \(\neq\) \(\neq\) SU(2) algebras associated with the holons of \(\eta\) spin 1/2 and spinons of spin 1/2, respectively, of both representations.

Next, let us consider the transport of charge and spin within the two alternative representations. The electronic charge and spin remain invariant under the electron - rotated-electron unitary transformation and thus the rotated electrons have the same charge and spin as the electrons 29. Thus, it follows from the relation of the rotated electrons to the \(-1/2\) holons and \(+1/2\) holons that the latter objects carry charge \(-2e\) and \(+2e\), respectively. However, within the pseudofermion representation only the \(-1/2\) holons of charge \(-2e\) are active charge carriers for the description of the charge transport in terms of electrons. In turn, for the description of the charge transport in terms of electronic holes, only the \(+1/2\) holons of charge \(+2e\) are active charge carriers. The charge is also carried by the \(c\) pseudofermions, which describe the charge degrees of freedom of the lattice sites singly occupied by rotated electrons. As discussed in Refs. 2330, for the description of the charge transport in terms of electrons (and electronic holes) the \(c\) pseudofermions carry charge \(-e\) and \(+e\). (Such objects have no spin and \(\eta\)-spin degrees of freedom.) We recall that the \(c\) \(\neq c\) pseudofermions (and \(s\) \(\neq s\) pseudofermions) are \(\eta\)-spin zero (and spin zero) composite objects of an equal number \(\nu = 1, 2, \ldots\) of \(-1/2\) holons and \(+1/2\) holons (and \(-1/2\) spinons and \(+1/2\) spinons). Thus, within the
description of charge transport in terms of electrons (and electronic holes), the \(c\nu\) pseudofermions carry charge \(-2\nu e\) (and \(+2\nu e\)) where \(\nu = 1, 2, \ldots\).

The charge \(-e\) carried by the \(\Delta N\) electrons (or the charge \(+e\) carried by the \(\Delta N^h\) electronic holes) involved in a transition from the ground state to an excited state is distributed by the objects of the pseudofermion representation as given in Eq. (57) of Ref. 29. Also the electronic spin remains invariant under the electron - rotated-electron unitary transformation. Thus, within the pseudofermion representation, the deviations \(\Delta N_{\uparrow}\) and \(\Delta N_{\downarrow}\) in the numbers of electronic up and down spins, respectively, are distributed by the quantum objects as 

\[
\Delta N_{\uparrow} = \Delta M_{s, +1/2} + \Delta M_{c, -1/2} = \sum_{\nu=1}^\infty \nu \Delta N_{s\nu} + \Delta L_{c, +1/2} + \Delta L_{c, -1/2}
\]

\[
\Delta N_{\downarrow} = \Delta M_{s, -1/2} + \Delta M_{c, 1/2} = \sum_{\nu=1}^\infty \nu \Delta N_{s\nu} - \Delta L_{c, -1/2} + \Delta L_{c, +1/2}.
\]

Note that in addition to the spinons, which correspond to the electronic spins of the rotated-electron singly occupied sites, some of the electronic spins refer to the rotated-electron doubly occupied sites. The latter electronic spins are contained in the \(-1/2\) holons. Each of these objects corresponds to one spin-zero on-site pair of rotated electrons with opposite spin projection. Thus, in spite of the \(-1/2\) holon being a spin-zero object, it contains one electronic up spin and one electronic down spin. It follows that one \(c\nu \neq c0\) pseudofermion, which is a composite object of \(\nu -1/2\) holons and \(\nu +1/2\) holons, contains \(\nu\) electronic up spins and \(\nu\) electronic down spins. In spite of the Yang holons having charge and the HL spinons spin, such objects have a localized character and thus do not contribute to the transport of charge and spin, respectively.

For the extended spinon-holon theory the holons and spinons are behind the transport of charge and spin, respectively. The holons of that theory carry half of the charge of those of the pseudofermion representation. Thus, such \(-1/2\) holons and \(+1/2\) holons carry \(-e\) and \(+e\), respectively.

Moreover, while for the pseudofermion representation the \(-1/2\) holons and \(+1/2\) holons correspond to alternative descriptions of the charge transport in terms of electrons and electronic holes, respectively, for the extended spinon-holon theory the charge transport is performed at the same time by the \(-1/2\) holons and \(+1/2\) holons. Indeed, it follows from Eq. (35) that for the latter theory one has that 

\[
(-e) \Delta N = (-e) \Delta M_{c, -1/2} + (+e) \Delta M_{c, +1/2}.
\]

Furthermore, concerning the spin transport it also follows from Eq. (35) that 

\[
\Delta N_{\uparrow} - \Delta N_{\downarrow} = \Delta M_{s, +1/2} - \Delta M_{s, -1/2}.
\]

In conclusion, the two alternative representations associated with the scattering theories of Refs. 18, 19 and 22, 23, 24, respectively, are faithful. However, such scattering theories refer to two alternative choices of one-particle scattering states, scatterers, scattering centers, and carriers of charge and spin.

### B. THE EXTENDED SPINON-HOLON THEORY AND SUITABILITY FOR THE DESCRIPTION OF THE FINITE-ENERGY SPECTRAL AND DYNAMICAL PROPERTIES

For the extended spinon-holon scattering theory the scatterers and (scattering centers) are the holons and spinons of the excited energy eigenstates associated with the one-particle scattering states (and the holons and spinons created under the corresponding ground-state - excited-state transitions). (Since the initial ground state of the reduced subspace considered in Sec. III and Refs. 22, 23, 24 has no holons and no spinons, all holons and spinons of the corresponding excited states are both scatterers and scattering centers.) Furthermore, for the extended spinon-holon representation the number of holons and spinons equals the number of \(c0\) pseudofermion holes and \(s1\) pseudofermion holes, respectively, of the pseudofermion representation. As for the reduced-subspace holon and spinon phase shifts studied in Sec. III, the holon-scatterer and spinon-scatterer phase shifts of the extended spinon-holon theory equal the corresponding phase shifts of the \(c0\) pseudofermion holes and \(s1\) pseudofermion holes, respectively. The many-particle states associated with the one-particle scattering states of that extended theory can always be expressed in terms of the excited energy eigenstates associated with the corresponding one-pseudofermion scattering states, as we have illustrated in Sec. III for the reduced subspace. As for that reduced subspace, many of the one-particle scattering states of the extended spinon-holon theory do not correspond to \(\eta\)-spin and spin eigenstates. On the other hand, the scattering states of such an extended scattering theory always refer to eigenstates of the \(\eta\)-spin and spin projections, but for initial ground states with densities in the ranges \(0 < n < 1\) and \(0 < m < n\) many of these states do not correspond to energy and momentum eigenstates. The many-particle states and associated one-particle scattering states of the two representations have the following general properties:

1. All one-pseudofermion scattering states correspond to excited energy and momentum eigenstates;

2. All excited many-particle states of one-particle scattering states of the extended spinon-holon theory whose expressions in terms of the excited energy eigenstates do not involve states with finite occupancy of \(\alpha\nu\) pseudofermions belonging to \(\alpha\nu \neq c0\), \(s1\) branches are energy and momentum eigenstates;
3. For initial ground states with electronic density \( n = 1 \) (and spin density \( m = 0 \)) all excited many-particle states of one-particle scattering states of the extended spinon-holon theory whose expressions in terms of the excited energy eigenstates involve states with finite occupancy of \( \alpha \nu \) pseudofermions belonging to \( \nu \neq c \) branches (and \( \nu \neq s \) branches) are energy eigenstates;

4. For initial ground states with electronic densities in the range \( 0 < n < 1 \) (and spin densities in the range \( 0 < m < n \)) the excited many-particle states of one-particle scattering states of the extended spinon-holon theory whose expressions in terms of the excited energy eigenstates involve states with finite occupancy of \( \alpha \nu \) pseudofermions belonging to \( \nu \neq c \) branches (and \( \nu \neq s \) branches) are not in general energy and momentum eigenstates;

These properties refer to the Hamiltonian \( \hat{H} \) of Eq. (1), whose excited-state energy is measured relative to that of the initial ground state, as for the PDT spectral-function expressions (15, 16). (Property 3 is valid when for initial ground states with electronic density \( n = 1 \) the zero-energy level corresponds to the middle of the Mott-Hubbard gap.) As a simple example, let us consider that the initial ground state has an electronic density in the range \( 0 < n < 1 \) and such that \( N \) is even and \( N_\uparrow \) and \( N_\downarrow \) are odd. In contrast to the \( n = 1 \) ground state, the \( \nu \neq c \) band of such a state is occupied by \( \nu \neq c \) pseudofermion holes for bare-momentum values in the range \( 2k_F < |q| < \pi \). Let us consider four excited energy eigenstates whose \( \nu \neq c \) pseudofermion occupancy configuration differs from that of the initial ground state by the creation of two \( \nu \neq c \) pseudofermion holes at given fixed bare momentum values \( q_1 \) and \( q_2 \) in the range \( q_1, q_2 \in [-2k_F, +2k_F] \) and such that \( q_1 \neq q_2 \). These four excited states are a generalization for \( n < 1 \) of the set of four excited states of the \( n = 1 \) ground state including the three \( \eta \) spin-triplet excited states and the \( \eta \) spin singlet excited state considered in Sec. III. As in that section, for each of the two alternative representations we replace the one-particle state under consideration by a suitable many-particle excited state with the same eigenvalue for the one-particle \( S \) operator and thus with the same value for the one-particle \( S \) matrix. Within the pseudofermion representation we again denote the above four states by \( |c, 0, 0, \eta \rangle \), \( |c, 0, \eta \rangle \), \( |\eta, 0, 0 \rangle \), \( |\eta, 0, \eta \rangle \), and \( |\eta, 0, +1 \rangle \) where the branch indices refer to the quantum objects created under the corresponding ground-state - excited-state transition. These four many-pseudofermion states correspond to four one-pseudofermion scattering states whose scatterer is a \( \nu \neq c \) pseudofermion hole. For electronic densities \( n < 1 \) one has that the index with values \( 0, \pm 1 \) refers to the \( \eta \) spin projection deviation \( \Delta S^z \) of the excited states, rather than to \( S^z \). Indeed, the \( n < 1 \) initial ground state has a finite value for the \( \eta \) spin projection. Another important difference is that the \( 1 \) pseudofermion scattering center of the excited state \( |\eta, 0, 0, 0 \rangle \) can be created under the ground-state - excited-state transition for bare-momentum values in the range \( q_3 \in [-(\pi - 2k_F), +\pi - 2k_F)] \) and has a \( q_3 \) dependent energy dispersion, plotted in Figs. 8 and 9 of Ref. 32.

At fixed values of \( q_1, q_2, \) and \( q_3 \) there are for the extended spinon-holon theory four one-particle scattering states which correspond to four well-defined excited many-particle states. As in Sec. III we denote the latter states by \( | 1/2, 1/2, +1/2, c \rangle, | 1/2, 1/2, -1/2, c \rangle, | -1/2, 1/2, +1/2, c \rangle, \) and \( | -1/2, -1/2, c \rangle \). They correspond to the above four excited energy eigenstates. (We recall that the relation of such bare-momentum values to the quantum numbers of the equations introduced by Takahashi is defined by Eqs. (A.1) and (B.1) of Ref. 29.) The \( n < 1 \) initial ground state has a finite occupancy of holons corresponding to \( \nu \) values of the BA distribution of \( k \)’s excitation spectrum in the range \( Q < |k| < \pi \). However, the two holons associated with the \( \eta \) spin state indices of these excited states are those created under the ground-state - excited-state transitions at \( k_1 = k^0(q_1) \) and \( k_2 = k^0(q_2) \) in the range \( k_1, k_2 \in [-Q, +Q] \) with \( k_1 \neq k_2 \). Here \( k^0(q) \) is the rapidity function defined by the first equation of Eq. (A.1) of Ref. 15 and the \( \nu \) Fermi value \( Q \) is the parameter introduced in Ref. 14, which is related to the \( \nu \) bare-momentum \( \nu \) Fermi value \( 2k_F \) by Eq. (A.5) of Ref. 15. As for \( n = 1 \), one finds that the four many-particle excited states associated with the holon-holon one-particle scattering states of the extended spinon-holon theory have in terms of the corresponding excited energy eigenstates associated with the one-pseudofermion scattering states expressions similar to those of Eq. 32 for \( \alpha = c, \alpha \nu = \nu \), and \( \alpha \nu' = c \). For initial ground states with electronic density \( n < 1 \) the excited energy eigenstates \( |c, 0, 0; 0 \rangle \) and \( |0, 0, 0, 0 \rangle \) have not the same energy and thus the excited states \( | 1/2, 1/2, c \rangle \) and \( | -1/2, 1/2, c \rangle \) associated with the holon-holon one-particle scattering states are not energy eigenstates. Moreover, for \( n < 1 \) initial ground states the energy and momentum expectation values of these two excited states are different from the energy and momentum of the first and fourth excited states of Eq. 32. Indeed, for \( n < 1 \) there is no \( \eta \) spin \( SU(2) \) rotation symmetry, in contrast to the \( n = 1 \) case considered in Refs. 22, 21. It follows that for \( n < 1 \) the energy and momentum expectation values of the second and third excited states of Eq. 32 are not determined by the energy and momentum values of the two involved holons only: the length-one charge rapidity also contributes to these expectation values through its energy dispersion, which is a function of the bare-momentum value \( q_1 \). (See Figs. 8 and 9 of Ref. 32.) In contrast, for the pseudofermion scattering theory the \( c \) pseudofermion created under the ground-state - excited-state transition is an independent scattering center and scatterer in its own right, just as the two created \( c \) pseudofermion holes. Indeed, for the pseudofermion representation the excited energy eigenstate denoted here by \( |c, 0, 0, 0, 0 \rangle \) also contains a one-pseudofermion state whose scatterer is the \( c \) pseudofermion.
A similar analysis could be performed for a generalization of the spin triplet and singlet excited states considered in Sec. III (two-spinon states, within the extended spinon-holon representation) with a $m > 0$ initial ground state, as well as for any other PS excited states involving the creation of a finite number of $\alpha\nu \neq c\ell$, $s1$ pseudofermions.

Finally, let us discuss the suitability for applications to the study of the finite-energy spectral and dynamical properties of the two alternative scattering theories. For the $n < 1$ metallic phase it is desirable for the study of these properties that all one-particle scattering states correspond to energy eigenstates. This allows the use of suitable Lehmann representations for the spectral functions $\mathcal{P}_{\nu}$. However, only for the reduced subspace considered in Sec. III corresponding to the $n = 1$ Mott-Hubbard insulator initial ground state, all one-particle scattering states of the extended spinon-holon theory refer to energy eigenstates. Unfortunately, for initial ground states with electronic density in the range $0 < n < 1$ (and spin density in the range $0 < m < n$) there are for such an extended theory many one-particle scattering states which do not refer to energy and momentum eigenstates. Thus, Lehmann representations for the spectral functions as those used in the PDT of Refs. [15, 16] cannot be used for the metallic phase in the case of the extended spinon-holon scattering theory. In contrast, such a problem does not occur for the one-pseudofermion scattering states, which for the whole PS and all density values always correspond to excited energy and momentum eigenstates. For the $n = 1$ and $m = 0$ initial ground state of the reduced subspace considered in Sec. III the one-particle scattering states of the spinon-holon representation refer to eigenstates. However, since the scatterers and scattering centers of that theory have $\eta$-spin 1/2 or spin 1/2, the SO(4) symmetry implies that the $S$ matrix has a Yang Baxter Equation (YBE) like factorization, as the BA bare $S$ matrix of the original spin 1/2 electrons, instead of the stronger commutative factorization of the pseudofermion and hole $S$ matrix. The $S$ matrix [22] has indeed such a property [22, 23, 24].

Another advantage of the pseudofermion scattering theory of Refs. [18, 19] for applications to the study of the dynamical properties is that the $S$ matrix of its scatterers has dimension one. Let us consider a $\alpha\nu$ pseudofermion scatterer of canonical momentum $\bar{q}$ and a $\alpha\nu'$ pseudofermion scattering center of canonical momentum $\bar{q}'$. Thus, the canonical-momentum values $\bar{q}$ and $\bar{q}'$ correspond to an “out” state and a virtual state, respectively. The corresponding pseudofermion anticommutators read

$$\{f_{\bar{q}, \alpha\nu}, f_{\bar{q}', \alpha\nu'}\} = \frac{\delta_{\alpha\nu, \alpha\nu'}}{N_{\alpha\nu}} \left[ S_{\alpha\nu}(q) \right]^{1/2} e^{-i(q-q')/2} \frac{\Im \left( \left[ S_{\alpha\nu}(q) \right]^{1/2} \right)}{\sin((q-q')/2)} ; \quad \{f_{\bar{q}, \alpha\nu}, f_{\bar{q}', \alpha\nu'}\} = \{f_{\bar{q}, \alpha\nu}, f_{\bar{q}', \alpha\nu'}\} = 0 . \quad (41)$$

Note that the first pseudofermion anticommutation relation can be expressed solely in terms of the difference $[\bar{q} - \bar{q}']$ and the $S$ matrix of the excited-state $\alpha\nu$ pseudofermion scatterer. Following the results of Ref. [18], the one- and two-electron matrix elements between the initial ground state and the excited energy eigenstates can be expressed in terms of the anticommutators [41]. Thus, within the pseudofermion representation the $S$ matrix $S_{\alpha\nu}(q)$ given in Eq. (12) controls the spectral properties of the model. If it had dimension larger than one, the problem would be much more involved. This is the case of the spinon-holon scattering theory of Refs. [22, 23, 24], whose scatterers and scattering centers are spin 1/2 spinons and $\eta$-spin 1/2 holons. As shown in Sec. III for the reduced subspace, the corresponding spinon-spinon and holon-holon $S$ matrices are indeed non-diagonal and thus the problem of the evaluation of these matrix elements is much more complex for the spinon-holon representation.

Such a problem simplifies for the pseudofermion representation because the PS subspaces associated with a given one- or two-electron spectral function can be expressed in terms of direct products corresponding to each of the $\alpha\nu$ pseudofermion occupancy configurations of branches with finite pseudofermion occupancy [15, 17]. For these matrix elements the direct product is associated with the commutative factorization of the $S$ matrices provided in Eq. (12) in terms of the elementary $S$ matrices $S_{\alpha\nu, \alpha\nu'}(q_j, q_j')$, Eq. (13). Such commutativity is stronger than the symmetry associated with the YBE and results from the elementary $S$ matrices $S_{\alpha\nu, \alpha\nu'}(q_j, q_j')$ being simple phase factors, instead of matrices of dimension larger than one. The commutative factorization of the $S$ matrix occurs when the one-particle scattering states correspond to energy eigenstates and the scatterers and scattering centers are $\eta$-spin-neutral and/or spin-neutral, as occurs for the pseudofermion scattering theory [19]. Unfortunately, for initial ground states with densities in the ranges $0 < n < 1$ and $0 < m < n$ many one-particle scattering states of the extended spinon-holon theory do not refer to energy eigenstates. For these states the occupancy configurations of the BA charge (and spin) string excitations of length $\nu = 1, 2, ..., (and \nu = 2, 3, ...) are included in the holon (and spinon) scatterers and scattering centers so that the corresponding BA string branches lose their independent character. Thus, for the extended spinon-holon theory the above PS subspaces are expressed as the direct product of two subspaces only, referring to the holon and spinon occupancy configurations, respectively. It is this property of the extended spinon-holon theory that increases the complexity of the evaluation of the spectral functions for the metallic phase. Indeed, such a direct product does not include the BA charge and spin string excitations of length $\nu$ as independent branches, corresponding to independent scatterers and scattering centers. In contrast, within the pseudofermion representation such BA charge (and spin) string excitations of length $\nu = 1, 2, ..., (and \nu = 2, 3, ...)$ refer to independent $c\nu$ pseudofermion-scatterer (and $s\nu$ pseudofermion-scatterer) branches which exist in their own
right. The corresponding $c\nu$ pseudofermion (and $s\nu$ pseudofermion) occupancy configurations refer to independent subspaces which contribute to the direct product of the whole PS subspace relevant for the spectral function under consideration.

Last but not least, the holons (and spinons) of the extended spinon-holon representation always involve the quantum superposition of the degrees of freedom associated with the $c\nu$ pseudofermions and Yang holons (and $s\nu$ pseudofermions and HL spinons), which are not invariant and are invariant under the electron - rotated-electron unitary transformation, respectively. (When the holon-holon or spinon-spinon one-particle scattering states of the extended spinon-holon theory do not refer to energy eigenstates, the corresponding holons or spinons also involve the $c\nu \neq c\nu$ pseudofermion or $s\nu \neq s\nu$ pseudofermion occupancy configurations, respectively, as discussed above.) It follows that the holons (and spinons) of the extended spinon-holon representation are not invariant under that transformation. It turns out that the electron - rotated-electron unitary transformation plays a major role in the PDT of Refs. [13, 16]. For instance, the contribution of the Yang holons and HL spinons to the evaluation of the spectral functions by the PDT is considerably simplified by their invariance under that transformation. In contrast, the holon and spinon definition of the extended spinon-holon representation does not profit from the symmetries associated with such a unitary transformation, which renders impossible the use of key PDT procedures for the evaluation of the finite-energy one-electron and two-electron spectral functions.

V. CONCLUDING REMARKS

The quantum objects associated with the pseudofermion representation of Refs. [18, 19, 29] emerge naturally from the electron - rotated-electron unitary transformation. Such a transformation was shown in Ref. [29] to correspond to the first step performed by the exact diagonalization of the non-perturbative many-electron quantum problem. Therefore, the choice of quantum objects of Refs. [18, 19, 29] profits from the symmetries associated with the electron - rotated-electron unitary transformation. For instance, the holons and spinons are defined in such a way that they either remain invariant under that transformation (Yang holons and HL spinons) but then do not scatter or do not remain invariant under the same transformation and thus cannot exist as independent quantum objects.

Indeed, the holons (and spinons) that are not invariant under the electron - rotated-electron unitary transformation are always part of $2\nu$-holon (and $2\nu$-spinon) composite $\eta$-spin singlet (and spin singlet) pseudofermions, where $\nu = 1, 2, \ldots$ gives the number of pairs of $+1/2$ holons and $-1/2$ holons (and $+1/2$ spinons and $-1/2$ spinons). Interestingly, in the pseudofermion scattering theory the relation of the composite $c\nu$ pseudofermion (and $s\nu$ pseudofermion) scatterers and scattering centers to the holons (and spinons) has similarities with that of the physical particles to the quarks in chromodynamics [40]. Within the latter theory all quark composite physical particles must be color-neutral, yet the quarks have color. On the other hand, in the pseudofermion scattering theory all $2\nu$-holon (and $2\nu$-spinon) composite pseudofermion scatterers and scattering centers must have zero $\eta$-spin (and spin) and thus must be $\eta$-spin-neutral (and spin-neutral), yet the holons (and spinons) have finite $\eta$-spin $1/2$ (and spin $1/2$). (The $c0$ pseudofermion scatterers and scattering centers are not composed of holons or spinons but are $\eta$-spin-less and spin-less objects.) In turn, the Yang holons and HL spinons have finite $\eta$-spin $1/2$ and spin $1/2$, respectively, but do not scatter.

As discussed above, it is precisely the $\eta$-spin-neutral (and spin-neutral) character of the $2\nu$-holon (and $2\nu$-spinon) composite pseudofermion scatterers and scattering centers and the $\eta$-spin-less and spin-less character of the $c0$ pseudofermion scatterers and scattering centers which is behind the dimension of their $S$ matrix $S_{\alpha\nu}(q_j)$ given in Eq. (12). We emphasize that such a $S$ matrix fully controls the pseudofermion anticommutators through Eq. (11) and also the value of the matrix elements between energy eigenstates and the corresponding finite-energy spectral properties, as confirmed by the studies of Refs. [15, 16]. Furthermore, within the pseudofermion representation all one-pseudofermion scattering states correspond to energy and momentum eigenstates.

Our study of the relation between the many-particle states associated with the one-particle scattering states of the conventional spinon-holon representation [22, 23, 24] and pseudofermion description [18, 19, 29], respectively, reveals that the $\eta$-spin $1/2$ holon and spin $1/2$ spinon scatterers and scattering centers of the former theory are different from the pseudofermion and pseudofermion-holone scatterers and scattering centers. The construction of the holon and spinon scatterers and scattering centers of the spinon-holon representation does not profit from the symmetries associated with the electron - rotated-electron unitary transformation. For instance, the holon and spinon scatterers and scattering centers of that theory involve mixing of the quantum objects of the pseudofermion representation that are not invariant under that transformation. It follows that many of the one-particle scattering states of the spinon- holon theory do not refer to $\eta$-spin and spin eigenstates and thus the corresponding holon-holon and spinon-spinon $S$ matrices are not diagonal. Moreover, for metallic initial ground states many of the one-particle scattering states of the extended spinon-holon theory do not correspond to energy and momentum eigenstates. As discussed in the previous section, these features of the extended spinon-holon representation imply that its use in the study of the finite-energy spectral and dynamical properties of the metallic phase is a much more involved problem than the use
of the pseudofermion scattering theory to study such properties.

Our investigation also reveals that both representations are faithful and thus that there is no inconsistency between the two corresponding definitions of quantum objects. The problem clarified in this paper is of interest for the further understanding of the unusual spectral properties observed in low-dimensional complex materials. Indeed, by use of the PDT of Refs. [12, 13], the unusual independent charge and spin finite-energy spectral features observed recently by angle-resolved photoelectron spectroscopy in quasi-1D metals [1] were shown in Ref. [2] to correspond to charge $c_0$ and spin $s_1$, respectively, pseudofermion-hole scatterers and scattering centers of the type considered in Refs. [13, 16]. (That such features correspond to charge and spin pseudofermions can be proved from the form of the $S$ matrix used in the evaluation of the one-electron matrix elements between the ground state and the excited states.) Thus, the exotic scatterers and scattering centers studied here and in these references exist in real low-dimensional complex materials. This indeed justifies the interest of clarifying their relation to the quantum objects of the conventional spinon-holon representation of Refs. [22, 23, 24, 31], which have been used in many theoretical studies of low-dimensional electronic correlated problems.

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APPENDIX A: USEFUL PHASE-SHIFT EXPRESSIONS

Here we provide expressions for phase shifts and other quantities needed for the evaluation of the overall phase shift given in Eq. (11). We start by providing the general expression for the overall scatter-less phase shift $Q^0_{c\nu}$ on the right-hand side of Eq. (11). It is given by [19],

\[ Q^0_{c\nu} = 0; \quad Q^0_{c\nu} = \pm \pi; \]

\[ Q^0_{c\nu} = 0; \quad Q^0_{c\nu} = \pm \pi; \quad Q^0_{c\nu} = \pm \pi; \]

\[ Q^0_{c\nu} = \pm \pi; \quad \Delta N_{c\nu} \quad \text{even}; \quad \Delta N_{c\nu} \quad \text{odd}; \]

\[ \Delta N_{c\nu} \quad \text{even}; \quad \Delta N_{c\nu} \quad \text{odd}; \quad \alpha = c, s, \nu > 0. \quad (A1) \]

When $Q^0_{c\nu} = \pm \pi$ for the $\alpha\nu \neq c\nu$ bands, the uniquely chosen and only permitted value $Q^0_{c\nu} = \pi$ or $Q^0_{c\nu} = -\pi$ is that which leads to symmetrical limiting discrete bare-momentum values $\pm[\pi/L][N^*_{c\nu} - 1]$ for the excited-state bare-momentum band. (See Eq. (B.14) of Ref. [25].) In turn, for the $c\nu$ branch the bare-momentum band width is $2\pi$. Thus, in this case $Q^0_{c\nu} = \pi$ and $Q^0_{c\nu} = -\pi$ lead to allowed occupancy configurations of alternative excited energy eigenstates. (In the particular case that the $c\nu$ band is full for the excited energy eigenstate, the two values $Q^0_{c\nu} = \pi$ and $Q^0_{c\nu} = -\pi$ refer to two equivalent representations of that state.)

In the remaining of this Appendix we provide quantities needed for the derivation of the overall phase-shift expressions (16)-(25). We start by providing the bare-momentum distribution function deviations for all types of excited states given by,

\[ \Delta N_{c\nu}(q) = -\frac{2\pi}{L} \sum_{l=1}^{2} \delta(q - q_{l}) - \frac{\pi}{L} \delta(q + \pi) + \frac{\pi}{L} \delta(q - \pi), \quad |q| \leq \pi; \quad \Delta N_{c1}(q) = -\frac{\pi}{L} \delta(q + \pi/2) - \frac{\pi}{L} \delta(q - \pi/2). \quad (A2) \]

The deviation $\Delta N_{c1}(q)$ given here also applies to the $\eta$-spin singlet excited states, whereas for the $c0$ and $c1$ branches the deviations read as follows for these states,

\[ \Delta N_{c0}(q) = -\frac{2\pi}{L} \sum_{l=1}^{2} \delta(q - q_{l}); \quad \Delta N_{c1}(q) = \delta q, 0. \quad (A3) \]

The three classes of spin triplet excited eigenstates considered in that section have the same expression for such deviations given by,

\[ \Delta N_{c0}(q) = -\frac{\pi}{L} \delta(q + \pi); \quad \Delta N_{c1}(q) = -\frac{2\pi}{L} \sum_{l=1}^{2} \delta(q - q_{l}^{*}) + \frac{\pi}{L} \delta(q + \pi/2) + \frac{\pi}{L} \delta(q - \pi/2), \quad |q| \leq \pi/2. \quad (A4) \]
The deviation $\Delta N_{c0}(q)$ given here also applies to the spin singlet excited states, whereas for the $s1$ and $s2$ branches the deviations read as follows for these states,

$$\Delta N_{s1}(q) = -\frac{2\pi}{L} \sum_{l=1}^{2} \delta(q - q'_l), \quad |q| \leq \pi; \quad \Delta N_{s2}(q) = \delta_{q, 0}. \tag{A5}$$

The four classes of doublet excited states have the same bare-momentum distribution function deviations given by,

$$\Delta N_{c0}(q) = -\frac{2\pi}{L} \delta(q - q'_s), \quad |q| \leq \pi; \quad \Delta N_{s1}(q) = -\frac{2\pi}{L} \delta(q - q'_s), \quad |q'_s| \leq \pi/2. \tag{A6}$$

Finally, we provide several two-pseudofermion phase-shift expressions needed for the derivation of the overall phase-shift expressions given in Eqs. (21)-(23). The rapidity two-pseudofermion phase shifts $2\pi \Phi_{\nu, \nu'}(r, r')$ are defined by the integral equations (A1)-(A13) of Ref. [30]. We solve these equations by Fourier transforming them after considering that $Q = \pi$ and $B = \infty$ and thus $r^0_c = 4t \sin Q/U = 0$ and $r^0_s = 4t B/U = \infty$ for finite values of $U/t$. Such a procedure leads to the following expressions valid for $n \rightarrow 1, m \rightarrow 0$, and finite values of $U/t$ for the two-pseudofermion phase shifts involving the $c0$ and $s1$ scatterers,

$$2\pi \Phi_{c0, c0}(r, r') = -2B(r - r'); \quad 2\pi \Phi_{c0, s1}(r, r') = -\arctan\left(\sinh\left(\frac{\pi}{2}(r - r')\right)\right), \tag{A7}$$

$$2\pi \Phi_{s1, c0}(r, r') = -\arctan\left(\sinh\left(\frac{\pi}{2}(r - r')\right)\right); \quad r \neq \pm \infty$$

$$= -\frac{\text{sgn}(r)\pi}{\sqrt{2}}; \quad r = \pm \infty, \tag{A8}$$

$$2\pi \Phi_{s1, s1}(r, r') = 2B(r - r'); \quad r \neq \pm \infty$$

$$= \frac{\text{sgn}(r)\pi}{\sqrt{2}}; \quad r = \pm \infty, \quad r' \neq r$$

$$= \left[\text{sgn}(r)\right]\left(3\sqrt{2} - 2\right)\pi; \quad r = r' = \pm \infty, \tag{A9}$$

$$2\pi \Phi_{c0, c1}(r, r') = -2\arctan(r - r'), \tag{A10}$$

$$2\pi \Phi_{s1, s2}(r, r') = 2\arctan(r - r'); \quad r \neq \pm \infty$$

$$= \pm\frac{2\pi}{\sqrt{2}}; \quad r = \pm \infty, \tag{A11}$$

and $2\pi \Phi_{c0, s2}(r, r') = 2\pi \Phi_{s1, c1}(r, r') = 0$. Here,

$$2B(r) = i \ln \frac{\Gamma\left(\frac{1}{2} + i\frac{r}{\pi}\right)\Gamma\left(1 - i\frac{r}{\pi}\right)}{\Gamma\left(\frac{1}{2} - i\frac{r}{\pi}\right)\Gamma\left(1 + i\frac{r}{\pi}\right)}. \tag{A12}$$

For the two types of excited states of Table I of Sec. III with one $c1$ pseudofermion and one $s2$ pseudofermion, respectively, the $n \rightarrow 1$ and $m \rightarrow 0$ equations $Q^c_{c1}(0) = 0$ and $Q^s_{c1}(0) = 0$ associated with the scatter-less character of such a pseudofermion can be written as $\sum_{l=1}^{2} \arctan(4t[\Lambda_{c1}(0) - \Lambda_{c1}^0(q'_l)])/U = 0$ and $\sum_{l=1}^{2} \arctan(4t[\Lambda_{s2}(0) - \Lambda_{s2}^0(q'_l)])/U = 0$, respectively [10]. Solution of these equations leads to $\Lambda_{c1}(0) = \Lambda_{c1}(0, q_1, q_2) = [\Lambda^0_{c1}(q_1) + \Lambda^0_{c1}(q_2)]/2$ and $\Lambda_{s2}(0) = \Lambda_{s2}(0, q'_1, q'_2) = [\Lambda^0_{s2}(q'_1) + \Lambda^0_{s2}(q'_2)]/2$, respectively. Use of that solution in the rapidity two-pseudofermion expressions of Eqs. (A10) and (A11) leads then to the following expressions for the two-pseudofermion phase shifts $2\pi \Phi_{c0, c1}(q_1, 0)$ and $2\pi \Phi_{s1, s2}(q'_1, 0)$ for $q'_1 \neq \pm \pi/2$,

$$2\pi \Phi_{c0, c1}(q_1, 0) = 2\pi \Phi_{c0, c1}\left(\frac{4t \Lambda^0_{c1}(q_1)}{U}, \frac{4t \Lambda_{c1}(0, q_1, q_2)}{U}\right) = -2\arctan\left(\frac{2t[\Lambda^0_{c1}(q_1) - \Lambda^0_{c1}(q_2)]}{U}\right); \tag{A13}$$

$$2\pi \Phi_{s1, s2}(q'_1, 0) = 2\pi \Phi_{s1, s2}\left(\frac{4t \Lambda^0_{s2}(q'_1)}{U}, \frac{4t \Lambda_{s2}(0, q'_1, q'_2)}{U}\right) = 2\arctan\left(\frac{2t[\Lambda^0_{s2}(q'_1) - \Lambda^0_{s2}(q'_2)]}{U}\right). \tag{A13}$$
