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General spectral function expressions of a 1D correlated model

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Abstract. We introduce a method that allows the evaluation of general expressions for the spectral functions of the one-dimensional Hubbard model for *all* values of the on-site electronic repulsion U. The spectral weights are expressed in terms of pseudofermion operators such that the spectral functions can be written as a convolution of pseudofermion dynamical correlation functions. Our results are valid for *all* finite energy and momentum values and are used elsewhere in the study of the unusual finite-energy properties of quasi-one-dimensional compounds and the new quantum systems of ultra-cold fermionic atoms on an optical lattice.

PACS. 71.10.Fd Lattice fermion models (Hubbard model, etc.) – 71.27.+a Strongly correlated electron systems; heavy fermions

1 Introduction

The main goal of this paper is to provide a general method for the evaluation of matrix elements of one-, two-electron, or $\mathcal{N}$-electron operators such that $\mathcal{N}$ is finite, between the ground state and excited energy eigenstates of the one-dimensional (1D) Hubbard model. Our results correspond to an important part of the derivation of the one-electron and two-electron spectral-weight distributions used in references [1,2] in the study of the phase diagram and unusual one-electron spectral properties of quasi-1D compounds. Indeed, the matrix-element and general spectral-function expressions derived here are used in reference [3] in the evaluation of closed-form expressions for the finite-energy one-electron and two-electron spectral-weight distributions of the model metallic phase. The studies of reference [4] confirm that such expressions lead to the known correct results in the limit of low energy. The 1D Hubbard model is one of the few realistic models for which one can exactly calculate all the energy eigenstates and their energies [5,6]. In addition to the applications to the study of the unusual properties of the quasi-1D compounds presented in references [1,2], our results are also of interest for the understanding of the spectral properties of the new quantum systems described by ultra-cold fermionic atoms in optical lattices with on-site repulsion [7].

The electron–rotated-electron unitary transformation [8] introduced in reference [9] for all values of the on-site repulsion U and the pseudofermion scattering theory considered in reference [10] play a central role in the construction of the *pseudofermion dynamical theory* introduced here. The studies of reference [11] reveal that there is no inconsistency between such a scattering theory and that corresponding to the conventional spinon-holon representation of reference [12]. For finite values of U very little is known about the finite-energy spectral properties of the model. This is in contrast to simpler models [13]. Unfortunately, combination of the model Bethe-ansatz solution [5,6] with bosonization, conformal-field theory, or g-ology and Renormalization Group [14,15] only allows the derivation of low-energy correlation-function expressions. In the limit of infinite U the spectral functions can be evaluated by the method presented in reference [16] and there are recent numerical results for finite values of U [17], but it is difficult to extract from them information about the microscopic processes that control the unusual spectral properties of the model.

The paper is organized as follows: In Section 2 we introduce the model and the spectral-function problem and summarize the pseudofermion operational description used in our study. In Section 3 we write the general spectral functions in terms of rotated-electron operators. The

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description of the rotated-electron elementary processes in terms of pseudofermion operators is the problem addressed in Section 4. In Section 5 we express the spectral functions as a convolution of pseudofermion spectral functions and study the pseudofermion determinants involved in the expressions of these functions. Finally, the concluding remarks are presented in Section 6.

2 The model, the spectral functions, and the pseudofermion description

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

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

$$\hat{H}_{SO(4)} = -t \sum_{j=1}^{N_a} \sum_{\sigma=\uparrow,\downarrow} \sum_{\delta=-1,+1} c^\dagger_{j,\,\sigma}\, c_{j+\delta,\,\sigma} + U \sum_{j=1}^{N_a} [\hat{n}_{j,\uparrow} - 1/2][\,\hat{n}_{j,\downarrow} - 1/2]. \quad (1)$$

Here the operators $c^\dagger_{j,\,\sigma}$ and $c_{j,\,\sigma}$ are the spin-projection σ electronic creation and annihilation operators at site j and $\hat{n}_{j,\,\sigma} = c^\dagger_{j,\,\sigma}\, c_{j,\,\sigma}$ where $j = 1, 2, ..., N_a$. The number of lattice sites N_a is even and very large. We consider periodic boundary conditions. In the first expression of equation (1), $\mu_c = 2\mu$, $\mu_s = 2\mu_0 H$, μ_0 is the Bohr magneton, and the diagonal generators of the η-spin and spin $SU(2)$ algebras [18,19] $\hat{S}^c_z$ and $\hat{S}^s_z$, respectively, are given in equation (2) of reference [9]. The Hamiltonian $\hat{H}_{SO(4)}$ of equation (1) commutes with the six generators of these two algebras, their off-diagonal generators being given in equations (7) and (8), respectively, of reference [9]. The electron number operator reads $\hat{N} = \sum_\sigma \hat{N}_\sigma$, where $\hat{N}_\sigma = \sum_{j=1}^{N_a} \hat{n}_{j,\sigma}$. For simplicity, we use units such that the Planck constant and electronic lattice constant are one. The model (1) describes $N_\uparrow$ spin-up electrons and $N_\downarrow$ spin-down electrons in a chain of N_a sites, whose length in the units used here reads $L = N_a$. We introduce the Fermi momenta which, in the thermodynamic limit $L \rightarrow \infty$, are given by $\pm k_{F\sigma} = \pm\pi n_\sigma$ and $\pm k_F = \pm[k_{F\uparrow} + k_{F\downarrow}]/2 = \pm\pi n/2$, where $n_\sigma = N_\sigma/L$ and $n = N/L$. The electronic density can be written as $n = n_\uparrow + n_\downarrow$ and the spin density is given by $m = n_\uparrow - n_\downarrow$. We denote the η-spin value η and projection η_z (and spin value S and projection S_z) of an energy eigenstate by S_c and S^z_c (and S_s and S^z_s), respectively. The momentum operator reads,

$$\hat{P} = \sum_{\sigma=\uparrow,\downarrow} \sum_k \hat{N}_\sigma(k)\, k = \frac{L}{2\pi} \sum_{\sigma=\uparrow,\downarrow} \int_{-\pi}^{+\pi} dk\, \hat{N}_\sigma(k)\, k, \quad (2)$$

and commutes with the Hamiltonians given in equation (1). The spin-projection σ momentum distribution operator appearing in equation (2) is given by $\hat{N}_\sigma(k) = c^\dagger_{k,\,\sigma}\, c_{k,\,\sigma}$. Here $c^\dagger_{k,\,\sigma}$ and $c_{k,\,\sigma}$ are the spin-projection σ electron creation and annihilation operators of momentum k. These operators are related to the above local operators as follows,

$$c^\dagger_{k,\,\sigma} = \frac{1}{\sqrt{N_a}} \sum_{j=1}^{N_a} e^{+ikja}\, c^\dagger_{j,\,\sigma};$$

$$c_{k,\,\sigma} = \frac{1}{\sqrt{N_a}} \sum_{j=1}^{N_a} e^{-ikja}\, c_{j,\,\sigma}. \quad (3)$$

The Bethe-ansatz solvability of the 1D Hubbard model is restricted to the Hilbert subspace spanned by *regular states*, i.e. the lowest-weight states (LWSs) of the η-spin and spin algebras such that $S_\alpha = -S^\alpha_z$, where $\alpha = c,\, s$ [9]. For simplicity, in this paper we restrict our considerations to values of the electronic density n and spin density m such that $0 \leq n \leq 1$ and $0 \leq m \leq n$, respectively. Often our expressions are different for the $n = 1$ Mott-Hubbard insulator phase and $0 < n < 1$ metallic phase (and for $m = 0$ zero spin density and $0 < m < n$ finite spin densities).

The main aim of this paper is the evaluation of expressions for finite-ω $\mathcal{N}$-electron spectral functions $B^l_{\mathcal{N}}(k,\,\omega)$, such that $l = \pm 1$, of the general form,

$$B^l_{\mathcal{N}}(k,\,\omega) = \sum_f |\langle f|\, \hat{O}^l_{\mathcal{N}}(k)|GS\rangle|^2\, \delta\Big(\omega - l[E_f - E_{GS}]\Big); \quad l\omega > 0; \quad l = \pm 1, \quad (4)$$

where the operators in the matrix elements are such that,

$$\hat{O}^{+1}_{\mathcal{N}}(k) \equiv \hat{O}^\dagger_{\mathcal{N}}(k); \qquad \hat{O}^{-1}_{\mathcal{N}}(k) \equiv \hat{O}_{\mathcal{N}}(k). \quad (5)$$

Here the f summation runs over the excited energy eigenstates, the energies E_f correspond to these states, E_{GS} is the ground-state energy, and we use a momentum extended scheme such that $k \in (-\infty, +\infty)$. The operators $\hat{O}^\dagger_{\mathcal{N}}(k)$ and $\hat{O}_{\mathcal{N}}(k)$ carry momentum k and are denoted in equation (5) by $\hat{O}^l_{\mathcal{N}}(k)$ where $l = +1$ and $l = -1$, respectively. They are related to the local operators $\hat{O}^\dagger_{\mathcal{N},\,j} \equiv \hat{O}^{+1}_{\mathcal{N},\,j}$ and $\hat{O}_{\mathcal{N},\,j} \equiv \hat{O}^{-1}_{\mathcal{N},\,j}$, respectively, by a Fourier transform.

The local operators $\hat{O}^l_{\mathcal{N},\,j}$ can be written as a product of

$$\mathcal{N} = \sum_{l_c,\,l_s=\pm 1} \mathcal{N}^l_{l_c,\,l_s}; \quad l = \pm 1, \quad (6)$$

local electronic creation and annihilation operators. Here $\mathcal{N}^l_{l_c,\,l_s}$ is the number of local electronic creation and annihilation operators of the operator $\hat{O}^l_{\mathcal{N},\,j}$ for $l_c = -1$ and $l_c = +1$, respectively, and with spin down and spin up for $l_s = -1$ and $l_s = +1$, respectively. It is assumed that the ratio $\mathcal{N}/N_a$ vanishes in the thermodynamic limit. Note that, by construction, $\mathcal{N}^{+1}_{l_c,\,l_s}$ and $\mathcal{N}^{-1}_{l_c,\,l_s}$ are such that $\mathcal{N}^{+1}_{l_c,\,l_s} = \mathcal{N}^{-1}_{-l_c,\,l_s}$, $\mathcal{N}^{+1}_{-1,\,l_s} \geq \mathcal{N}^{+1}_{+1,\,l_s}$, and $\mathcal{N}^{-1}_{-1,\,l_s} \leq \mathcal{N}^{-1}_{+1,\,l_s}$. For $\mathcal{N} > 1$ the operator $\hat{O}^l_{\mathcal{N},\,j}$ has a well defined local structure involving the $\mathcal{N}_{-1,\,l_s}$ electronic creation operators of spin projection $l_s/2$, and

$\mathcal{N}^{l}_{+1,\,l_s}$ electronic annihilation operators of spin projection $l_s/2$ located in neighboring lattice sites. The more usual cases for the description of experimental studies correspond to $\mathcal{N}=1$ and $\mathcal{N}=2$. Examples of $\mathcal{N}$-electron operators $\hat{O}_{\mathcal{N}}(k)\equiv\hat{O}^{-1}_{\mathcal{N}}(k)$ are the one-electron operator $\hat{O}_1(k)=c_{k,\,\sigma}$ (measured in the angle-resolved photoelectron spectroscopy), the spin-projection σ density operator $\hat{O}^{\sigma sd}_2(k)=\frac{1}{\sqrt{N_a}}\sum_{k'}c^{\dagger}_{k+k',\,\sigma}c_{k',\,\sigma}$, the transverse spin-density operator $\hat{O}^{sdw}_2(k)=\frac{1}{\sqrt{N_a}}\sum_{k'}c^{\dagger}_{k+k',\,\uparrow}c_{k',\,\downarrow}$, the on-site s-wave singlet superconductivity operator $\hat{O}^{oss}_2(k)=\frac{1}{\sqrt{N_a}}\sum_{k'}c_{k-k',\,\uparrow}c_{k',\,\downarrow}$, and the spin-projection σ triplet superconductivity operator $\mathcal{O}^{\sigma ts}_2(k)=\frac{1}{\sqrt{N_a}}\sum_{k'}\cos(k')\,c_{k-k',\,\sigma}c_{k',\,\sigma}$. The corresponding local operators $\hat{O}^{-1}_{\mathcal{N},\,j}\equiv\hat{O}_{\mathcal{N},\,j}$ are $\hat{O}_{1,\,j}=c_{j,\,\sigma}$, $\hat{O}^{\sigma sd}_{2,\,j}=c^{\dagger}_{j,\,\sigma}c_{j,\,\sigma}$, $\hat{O}^{sdw}_{2,\,j}=c^{\dagger}_{j,\,\uparrow}c_{j,\,\downarrow}$, $\hat{O}^{oss}_{2,\,j}=c_{j,\,\uparrow}c_{j,\,\downarrow}$, and $\hat{O}^{\sigma ts}_{2,\,j}=c_{j,\,\sigma}c_{j+1,\,\sigma}$, respectively. The charge density operator (measured in density-density electron energy loss spectroscopy and inelastic X-ray scattering) is written in terms of the above spin-up and spin-down density operators. The operators $\hat{O}^{l}_{\mathcal{N}}(k)$ of physical interest, correspond in general to operators $\hat{O}^{l}_{\mathcal{N},\,j}$ whose $\mathcal{N}$ elementary electronic operators create or annihilate electrons in a compact domain of lattice sites. For instance, if $\hat{O}^{+1}_{2,\,j}=c^{\dagger}_{j,\downarrow}c^{\dagger}_{j+i,\uparrow}$ and thus $\hat{O}^{-1}_{2,\,j}=c_{j+i,\uparrow}\,c_{j,\downarrow}$, the interesting cases correspond to $i=0$ (on-site s-wave singlet superconductivity) and $i=1$ (extended s-wave singlet superconductivity).

The k dependence of the spectral functions (4) can be transferred from the $\mathcal{N}$-electron operators $\hat{O}^{l}_{\mathcal{N}}(k)$ to the excited energy eigenstates as follows,

$$B^{l}_{\mathcal{N}}(k,\,\omega)=\sum_{f}N_a|\langle f|\,\hat{O}^{l}_{\mathcal{N},\,0}|GS\rangle|^2\,\delta\Big(\omega-l[E_f-E_{GS}]\Big)\,\delta_{k,\,l[k_f-k_{GS}]};\quad l\omega>0;\quad l=\pm1. \tag{7}$$

Here, $\hat{O}^{l}_{\mathcal{N},\,0}$ is the $j=0$ local operator $\hat{O}^{l}_{\mathcal{N},\,j}$ considered above, k_f is the momentum of the excited energy eigenstates, and k_{GS} denotes the ground-state momentum. In this expression, we have chosen $j=0$ for the local operator $\hat{O}^{l}_{\mathcal{N},\,j}$. Due to translational invariance, the value of the functions (7) is independent of this special choice.

Let us summarize the basic information about the holon, spinon, pseudoparticle, and pseudofermion descriptions needed for our studies. (For further information, see Refs. [3,4,9,20,21].) These studies involve the electron–rotated-electron unitary transformation, such that rotated-electron double occupancy is a good quantum number for all U/t values [9]. As the Fermi-liquid quasiparticles, the rotated electrons have the same charge and spin as the electrons, but refer to all energies and reorganize in terms of $[N_a-N_c]$ η-spin 1/2 holons, N_c spin 1/2 spinons, and N_c spinless and η-spinless c pseudoparticles, where N_c is the number of rotated-electron singly occupied sites [9]. We use the notation $\pm1/2$ holons and $\pm1/2$ spinons, which refers to the η-spin and spin projections, respectively. The $\pm1/2$ holons of charge $\pm2e$ correspond to rotated-electron unoccupied (+) and doubly-occupied (−) sites. The complex behavior occurs for the spin-projection σ-rotated electrons occupying singly occupied sites: their spin degrees of freedom originate chargeless spin-projection σ spinons, whereas their charge part gives rise to η-spinless and spinless c pseudoparticles of charge $-e$.

Based on symmetry considerations, we can classify the $\pm1/2$ holons and $\pm1/2$ spinons into two classes: those which remain invariant under the electron–rotated-electron unitary transformation, and those which do not. The former are called independent $\pm1/2$ holons and independent $\pm1/2$ spinons. For instance, the $\pm1/2$ Yang holons and $\pm1/2$ HL spinons [3,9,20,21] with numbers reading $L_{c,\,\pm1/2}=[S_c\mp S^z_c]$ and $L_{s,\,\pm1/2}=[S_s\mp S^z_s]$, respectively, belong to the former group of holons and spinons. The latter are part of η-spin-zero 2ν-holon composite $c\nu$ pseudoparticles and spin-zero 2ν-spinon composite $s\nu$ pseudoparticles, respectively, where $\nu=1,2,...$ is the number of $+1/2$ and $-1/2$ holon or $+1/2$ and $-1/2$ spinon pairs. Thus, the total number of $\pm1/2$ holons ($\alpha=c$) and $\pm1/2$ spinons ($\alpha=s$) reads $M_{\alpha,\,\pm1/2}=L_{\alpha,\,\pm1/2}+\sum_{\nu=1}^{\infty}\nu\,N_{\alpha\nu}$, where $N_{\alpha\nu}$ denotes the number of composite $\alpha\nu$ pseudoparticles. The total number of holons ($\alpha=c$) and spinons ($\alpha=s$) is then given by $M_\alpha=L_\alpha+2\sum_{\nu=1}^{\infty}\nu\,N_{\alpha\nu}$ where $L_\alpha=2S_\alpha$ denotes the total number of Yang holons ($\alpha=c$) and HL spinons ($\alpha=s$). These numbers are such that $M_c=[N_a-N_c]$ and $M_s=N_c$. The pseudoparticles can be defined in terms of bare-momentum or spatial coordinates [9]. In addition to the Yang holons and HL spinons, also the holons and spinons associated with $\alpha\nu\neq c0,\,s1$ pseudoparticles of limiting bare-momentum values $\pm q_{\alpha\nu}$ are independent holons and spinons. ($q_{\alpha\nu}$ is given in Eq. (B.14) of Ref. [9].) Indeed, the invariance under the electron–rotated-electron unitary transformation of such $c\nu$ pseudoparticles (and $s\nu$ pseudoparticles) implies that they separate into 2ν independent holons (and 2ν independent spinons) and a $c\nu$ (and $s\nu$) FP current scattering center [10]. (These centers are defined in the second paper of Ref. [10].) The emergence of the exotic quantum phases of matter considered in our study involves a second unitary transformation, which maps the c pseudoparticles (and composite $\alpha\nu$ pseudoparticles) onto c pseudofermions (and composite $\alpha\nu$ pseudofermions) [3]. Such a transformation introduces shifts of order $1/L$ in the pseudoparticle discrete momentum values and leaves all other pseudoparticle properties invariant. Here we use the designation $c0$ pseudoparticle and pseudofermion for the c pseudoparticle and pseudofermion, respectively. Thus, the $c\nu$ and $s\nu$ branches are such that $\nu=0,1,2,...$ and $\nu=1,2,...$, respectively.

The local $\alpha\nu$ pseudofermion creation (and annihilation) operator $f^{\dagger}_{x_j,\,\alpha\nu}$ (and $f_{x_j,\,\alpha\nu}$) creates (and annihilates) a $\alpha\nu$ pseudofermion at the effective $\alpha\nu$ lattice site of spatial coordinate $x_j=j\,a^0_{\alpha\nu}$. Here $j=1,2,...,N^*_{\alpha\nu}$ and $a^0_{\alpha\nu}=L/N^*_{\alpha\nu}=N_a/N^*_{\alpha\nu}$ is the effective $\alpha\nu$ lattice constant introduced in reference [20] in units of the electronic

lattice constant. The general expression of the number of effective $\alpha\nu$ lattice sites $N^*_{\alpha\nu}$ is given in equation (B6) of reference [9], where the number of $\alpha\nu$ pseudofermion holes $N^h_{\alpha\nu}$ is provided in equation (B.11) of the same reference. (The number of pseudofermion and pseudofermion holes equals that of the corresponding pseudoparticle and pseudoparticle holes [3,20].) The operator $f^\dagger_{x_j,\,\alpha\nu}$ (and $f_{x_j,\,\alpha\nu}$) is related to the operator $f^\dagger_{\bar{q}_j,\,\alpha\nu}$ (and $f_{\bar{q}_j,\,\alpha\nu}$), which refers to $\alpha\nu$ pseudofermions of canonical-momentum $\bar{q}_j$, by a Fourier transform. The discrete canonical-momentum values of the $\alpha\nu$ pseudofermions have a functional character and read [3,10],

$$\bar{q}_j = q_j + Q^{\Phi}_{\alpha\nu}(q_j)/L = [2\pi/L]I^{\alpha\nu}_j + Q^{\Phi}_{\alpha\nu}(q_j)/L; \quad j = 1,2,...,N^*_{\alpha\nu}, \tag{8}$$

where $q_j = [2\pi I^{\alpha\nu}_j]/L$ [9] is the bare-momentum carried by the $\alpha\nu$ pseudoparticles. Here $I^{\alpha\nu}_j$ are the actual quantum numbers provided by the Bethe-ansatz solution [9]. Although the $\alpha\nu$ pseudoparticles carry bare-momentum q_j, one can also label the corresponding $\alpha\nu$ pseudofermions by such a bare-momentum. When one refers to the pseudofermion bare-momentum q_j, one means that q_j is the bare-momentum value that corresponds to the canonical momentum $\bar{q}_j = q_j + Q^{\Phi}_{\alpha\nu}(q_j)/L$. Here and in equation (8) $Q^{\Phi}_{\alpha\nu}(q_j)/2$ is a $\alpha\nu$ pseudofermion overall scattering phase shift given by [10],

$$Q^{\Phi}_{\alpha\nu}(q_j)/2 = \pi \sum_{\alpha'\nu'} \sum_{j'=1}^{N^*_{\alpha'\nu'}} \Phi_{\alpha\nu,\,\alpha'\nu'}(q_j, q_{j'})\, \Delta N_{\alpha'\nu'}(q_{j'}); \quad j = 1,2,...,N^*_{\alpha\nu}, \tag{9}$$

where $\Delta N_{\alpha\nu}(q_j) = \Delta\mathcal{N}_{\alpha\nu}(\bar{q}_j)$ is the distribution function deviation $\Delta N_{\alpha\nu}(q_j) = N_{\alpha\nu}(q_j) - N^0_{\alpha\nu}(q_j)$. The canonical-momentum distribution function $\mathcal{N}_{\alpha\nu}(\bar{q}_j)$ (and bare-momentum distribution function $N_{\alpha\nu}(q_j)$) is given by $\mathcal{N}_{\alpha\nu}(\bar{q}_j) = 1$ and $\mathcal{N}_{\alpha\nu}(\bar{q}_j) = 0$ (and $N_{\alpha\nu}(q_j) = 1$ and $N_{\alpha\nu}(q_j) = 0$) for pseudofermions and pseudofermion holes (and pseudoparticles and pseudoparticle holes), respectively [3]. The ground-state densely-packed bare-momentum distribution function $N^0_{\alpha\nu}(q_j)$ is defined in equations (C.1)–(C.3) of reference [9]. The $\alpha\nu \neq c0,\, s1$ pseudofermion limiting canonical-momentum values play an important role in the theory and read,

$$q^0_{\alpha\nu} = q_{\alpha\nu} + Q^{\Phi}_{\alpha\nu}(q_{\alpha\nu})/L; \quad \alpha\nu \neq c0,\, s1, \tag{10}$$

where $q^0_{\alpha\nu}$ is the ground-state limiting bare-momentum value given in equations (C.13) and (C.14) of reference [9] and $q_{\alpha\nu}$ the excited-energy-eigenstate limiting bare-momentum value provided in equation (B.14) of the same reference. In contrast to the $\alpha\nu$ pseudoparticles, the $\alpha\nu$ pseudofermions have no residual-interaction energy terms [3]. Instead, under the ground-state–excited-energy-eigenstate transitions the $\alpha\nu$ pseudofermions and $\alpha\nu$ pseudofermion holes undergo elementary scattering events with the $\alpha'\nu'$ pseudofermions and $\alpha'\nu'$ pseudofermion holes created in these transitions [10]. This leads to the elementary two-pseudofermion phase shifts $\pi\,\Phi_{\alpha\nu,\,\alpha'\nu'}(q_j, q'_j)$ on the right-hand side of the overall scattering phase shift (9), which are defined by a set of integral equations [3,10,20]. The overall $\alpha\nu$ pseudofermion or hole phase shift,

$$Q_{\alpha\nu}(q_j)/2 = Q^0_{\alpha\nu}/2 + Q^{\Phi}_{\alpha\nu}(q_j)/2, \tag{11}$$

plays an important role in the pseudofermion theory [3,10]. Here $Q^0_{\alpha\nu}/2$ can have the values $Q^0_{\alpha\nu}/2 = 0, \pm\pi/2$ [3,10].

The pseudofermion description refers to a Hilbert subspace called *pseudofermion subspace* (PS) where the $\mathcal{N}$-electron excitations are contained [3,10]. The PS is spanned by the initial ground state and the excited energy eigenstates generated from it by the following types of processes (A)–(C), which are defined in more detail in references [3,20]: (A) finite-energy and finite-momentum elementary $c0$ and $s1$ pseudofermion processes plus creation of $\alpha\nu \neq c0,\, s1$ pseudofermions with bare-momentum values $q \neq \pm q_{\alpha\nu}$; (B) zero-energy and finite-momentum processes that change the number of $c0$ and $s1$ pseudofermions at their *Fermi points*, which for the ground state and $L \rightarrow \infty$ read,

$$q^0_{Fc0} = 2k_F; \quad q^0_{Fs1} = k_{F\downarrow}, \tag{12}$$

plus creation of independent $-1/2$ holons and/or $-1/2$ spinons; and (C) low-energy and small-momentum elementary $c0$ and $s1$ pseudofermion particle-hole processes in the vicinity of the *Fermi points*. The PS contains subspaces of several CPHS ensemble subspaces. (Here CPHS stands for $c0$ pseudofermion, holon, and spinon.) A CPHS ensemble subspace is spanned by all energy eigenstates with fixed values for the $-1/2$ Yang holon number $L_{c,\,-1/2}$, $-1/2$ HL spinon number $L_{s,\,-1/2}$, $c0$ pseudofermion number N_{c0}, and for the sets of composite $\alpha\nu$ pseudofermion numbers $\{N_{c\nu}\}$ and $\{N_{s\nu}\}$ corresponding to the $\nu = 1,2,...$ branches.

The pseudofermion bare-momentum dependent energy dispersions $\epsilon_{c0}(q)$, $\epsilon_{s1}(q)$, $\epsilon_{c\nu}(q) = 2\nu\mu + \epsilon^0_{c\nu}(q)$ for $\nu > 0$, and $\epsilon_{s\nu}(q) = 2\nu\mu_0 H + \epsilon^0_{s\nu}(q)$ for $\nu > 1$, where $\mu = \mu(n)$ and $H = H(m)$ correspond to the density and magnetization curves, respectively, are defined and studied in references [3,9,21]. Such energy dispersions play a crucial role in the expressions of the $\mathcal{N}$-electron spectral functions. For $m = 0$, the energy 2μ is an increasing function of U and a decreasing function of the density n with the following limiting values,

$$\begin{aligned} 2\mu = {} & 4t\cos(\pi na/2), \quad U/t \rightarrow 0; \\ & U + 4t\cos(\pi na), \quad U/t \rightarrow \infty; \\ & U + 4t, \quad n \rightarrow 0; \\ & E_{MH}, \quad n \rightarrow 1, \end{aligned} \tag{13}$$

where E_{MH} is the half-filling Mott-Hubbard gap [5].

The evaluation of matrix elements between energy eigenstates considered in Section 5 involves pseudofermion operators $f^\dagger_{\bar{q},\,\alpha\nu}$ and $f_{\bar{q}',\,\alpha\nu}$ such that the canonical momentum values $\bar{q}$ and $\bar{q}' = q'$ correspond to an excited-energy-eigenstate and initial ground-state CPHS ensemble

subspaces, respectively. In that case the unusual pseudofermion anticommutation relations read [3,10],

$$\{f^{\dagger}_{\bar{q},\,\alpha\nu},\, f_{q',\,\alpha'\nu'}\} = \delta_{\alpha\nu,\,\alpha'\nu'}\,\frac{1}{N^{*}_{\alpha\nu}}\,e^{-i(\bar{q}-q')/2} \times e^{iQ_{\alpha\nu}(q)/2}\,\frac{\sin\Big(Q_{\alpha\nu}(q)/2\Big)}{\sin([\bar{q}-q']/2)}, \quad (14)$$

and $\{f^{\dagger}_{\bar{q},\,\alpha\nu},\, f^{\dagger}_{q',\,\alpha'\nu'}\} = \{f_{\bar{q},\,\alpha\nu},\, f_{q',\,\alpha'\nu'}\} = 0$.

3 Spectral functions in terms of rotated-electron operators

Here we express the general $\mathcal{N}$-electron spectral functions (7) in terms of rotated-electron creation and annihilation operators and evaluate the spectral-weight contributions from the Yang holons and HL spinons. Our first goal is identifying the set of CPHS ensemble subspaces which are spanned by the excited energy eigenstates generated by application onto the initial ground state of the operator $\hat{O}^{l}_{\mathcal{N},\,0}$ of equation (7). For clarification of this problem, we must find the set of deviation numbers ΔN_{c0}, ΔN_{s1}, $\{\Delta L_{\alpha,\,-1/2}\}$, and $\{\Delta N_{\alpha\nu}\}$ for $\alpha\nu \neq c0,\, s1$ that are generated by application onto the ground state of that operator. According to the results of references [3,9], for the ground state $M_{c,\,-1/2} = L_{\alpha,\,-1/2} = N_{\alpha\nu} = 0$ for the $\alpha\nu \neq c0,\, s1$ branches and thus $\Delta M_{c,\,-1/2} = M_{c,\,-1/2}$, $\Delta L_{\alpha,\,-1/2} = L_{\alpha,\,-1/2}$, and $\Delta N_{\alpha\nu} = N_{\alpha\nu}$ for the latter branches.

First, we note that the values of the $+1/2$ holon and $+1/2$ spinon number deviations are such that,

$$\begin{aligned}\Delta M_{c,\,+1/2} &= -\Delta N_{c0} - M_{c,\,-1/2};\\ \Delta M_{s,\,+1/2} &= \Delta N_{c0} - \Delta M_{s,\,-1/2},\end{aligned} \quad (15)$$

and thus are dependent on the values of the $-1/2$ holon and $-1/2$ spinon numbers and $c0$ pseudofermion number deviations. Also the occupancy configurations of the $-1/2$ holons and $-1/2$ spinons determine those of the $+1/2$ holons and $+1/2$ spinons. Indeed, the $-1/2$ holons and $+1/2$ holons correspond to the rotated-electron doubly-occupied sites and unoccupied sites, respectively, of a charge sequence. The point is that the spatial position of the unoccupied sites corresponds to the sites left over by the rotated-electron doubly occupied sites of a charge sequence. The same applies to the $-1/2$ spinons and $+1/2$ spinons, provided that we replace the rotated-electron doubly-occupied sites and unoccupied sites by sites singly occupied by spin-down and spin-up rotated electrons, respectively, and the charge sequence by the spin sequence. Moreover, the values of the corresponding $+1/2$ Yang holon and $+1/2$ HL spinon number deviations read,

$$\Delta L_{c,\,+1/2} = -\Delta N_{c0} - 2\sum_{\nu=1}^{\infty}\nu\,N_{c\nu} - L_{c,\,-1/2}, \quad (16)$$

and

$$\Delta L_{s,\,+1/2} = \Delta N_{c0} - 2\Delta N_{s1} - 2\sum_{\nu=2}^{\infty}\nu\,N_{s\nu} - L_{s,\,-1/2}, \quad (17)$$

respectively, and thus are not independent. One does not need to provide these values in order to specify a CPHS ensemble subspace. Therefore, often we do not consider in the expressions below the values of the holon numbers $M_{c,\,+1/2}$ and $L_{c,\,+1/2}$ and of the spinon numbers $M_{s,\,+1/2}$ and $L_{s,\,+1/2}$.

The values of the deviations $\Delta N_{\uparrow}$ and $\Delta N_{\downarrow}$ specific to a given $\mathcal{N}$-electron operator, lead to sum rules for the values of the number deviations of pseudofermions, $-1/2$ Yang holons, and $-1/2$ HL spinons as follows,

$$\Delta N = \Delta N_{c0} + 2L_{c,\,-1/2} + 2\sum_{\nu=1}^{\infty}\nu\,N_{c\nu}, \quad (18)$$

and

$$\Delta(N_{\downarrow} - N_{\uparrow}) = 2\Delta N_{s1} - \Delta N_{c0} + 2L_{s,\,-1/2} + 2\sum_{\nu=2}^{\infty}\nu\,N_{s\nu}. \quad (19)$$

Only transitions to excited energy eigenstates associated with deviations obeying the sum rules (18) and (19) are permitted. The same deviations are associated with sum rules obeyed by the numbers $\mathcal{N}^{l}_{l_c,\,l_s}$ of equation (6) for the operator $\hat{O}^{l}_{\mathcal{N},\,j}$ appearing in the general spectral-function expressions of equation (7). Such sum rules read,

$$\begin{aligned}\Delta N &= \sum_{l_c,\,l_s=\pm1}(-l_c)\,\mathcal{N}^{l}_{l_c,\,l_s};\\ \Delta(N_{\downarrow} - N_{\uparrow}) &= \sum_{l_c,\,l_s=\pm1}(l_c\,l_s)\,\mathcal{N}^{l}_{l_c,\,l_s}.\end{aligned} \quad (20)$$

Furthermore, it is straightforward to show that the following selection rule is valid for initial ground states corresponding to the density values considered in this paper: the values of the numbers of $-1/2$ Yang holons and $-1/2$ HL spinons generated by application onto the ground state of the $\mathcal{N}$-electron operator $\hat{O}^{l}_{\mathcal{N},\,j}$, equation (7), are restricted to the following ranges,

$$\begin{aligned}L_{c,\,-1/2} &= 0,1,2,...,\sum_{l_s=\pm1}\mathcal{N}^{l}_{-1,\,l_s};\\ L_{s,\,-1/2} &= 0,1,2,...,\sum_{l_c,\,l_s=\pm1}\delta_{l_c,\,l_s}\,\mathcal{N}^{l}_{l_c,\,l_s};\\ l &= \pm1,\end{aligned} \quad (21)$$

respectively. Here the numbers $\mathcal{N}^{l}_{l_c,\,l_s}$ are those of equation (6) specific to that operator.

Further selection rules in terms of the rotated-electron expressions for the operator $\hat{O}^{l}_{\mathcal{N},\,0}$ of the general spectral-function (7) are given in the ensuing section.

Let us label the excited energy eigenstates of the state summations of the general $\mathcal{N}$-electron spectral function (7) according to their CPHS ensemble subspace.

(We recall that all excited energy eigenstates belonging to a given CPHS ensemble subspace have the same values for the set of deviation numbers ΔN_{c0} and ΔN_{s1} and numbers $\{L_{\alpha,\,-1/2}\}$ for $\alpha = c,\, s$, and $\{N_{\alpha\nu}\}$ for the $\alpha\nu \neq c0,\, s1$ branches.) This procedure leads to the following expression for the spectral function (7),

$$B^{l}_{\mathcal{N}}(k,\,\omega) = \sum_{\{\Delta N_{\alpha\nu}\},\,\{L_{\alpha,\,-1/2}\}} \sum_{f} N_a |\langle f;\, C|\, \hat{O}^{l}_{\mathcal{N},\,0}|GS\rangle|^2 \times \delta\Big(\omega - l\Delta E_{cphs}\Big)\,\delta_{k,\,l\Delta k_{cphs}}; \quad l\omega > 0, \quad (22)$$

where $l = \pm 1$ and the summation $\sum_{\{\Delta N_{\alpha\nu}\},\,\{L_{\alpha,\,-1/2}\}}$ runs over the CPHS ensemble subspaces whose deviation values obey the sum rules (18) and (19) and selection rules (21). Moreover, the summation $\sum_{f}$ runs over the excited energy eigenstates $|f;\, C\rangle$ of a given CPHS ensemble subspace, ΔE_{cphs} is the excitation energy, and Δk_{cphs} the corresponding excitation momentum. A general energy eigenstate $|f\rangle$ with finite values for the numbers $L_{c,\,-1/2}$ and/or $L_{s,\,-1/2}$, can be expressed as follows,

$$|f\rangle = \prod_{\alpha=c,\,s} \frac{(\hat{S}^{\dagger}_{\alpha})^{L_{\alpha,\,-1/2}}}{\sqrt{\mathcal{C}_{\alpha}}}|f.L\rangle. \quad (23)$$

Here,

$$\mathcal{C}_{\alpha} = \delta_{L_{\alpha,\,-1/2},\,0} + \prod_{l=1}^{L_{\alpha,\,-1/2}} l\,[\,L_{\alpha} + 1 - l\,]; \quad L_{\alpha,\,-1/2} \leq L_{\alpha} = 2S_{\alpha}, \quad (24)$$

and the η-spin flip Yang holon ($\alpha = c$) and spin flip HL spinon ($\alpha = s$) operators $\hat{S}^{\dagger}_{\alpha}$ are the off-diagonal generators of the corresponding $SU(2)$ algebras given in equations (7) and (8), respectively, of reference [9]. These operators remain invariant under the electron–rotated-electron unitary transformation and thus have the same expression in terms of electronic and rotated-electron creation and annihilation operators. Moreover, in equation (23) $|f.L\rangle$ is the LWS that corresponds to the state $|f\rangle$. For a state $|f\,;C\rangle$ belonging to a given CPHS ensemble subspace the corresponding LWS is denoted by $|f.L\,;C\rangle$. However, note that a non-LWS $|f\,;C\rangle$ and the corresponding LWS $|f.L\,;C\rangle$ belong to different CPHSs, once they correspond to different values of the numbers $L_{c,\,-1/2}$ and/or $L_{s,\,-1/2}$.

It is useful to reexpress the spectral-function expression (22) in terms of matrix elements between regular states only. The ground state is a LWS of both the η-spin and spin $SU(2)$ algebras and thus has the following property,

$$\hat{S}_{\alpha}\,|GS\rangle = 0; \quad \alpha = c,\, s. \quad (25)$$

Let us introduce the operators $\hat{\Theta}^{l}_{\mathcal{N},\,j}$ and $\hat{\Theta}^{l}_{\mathcal{N},\,k}$ such that,

$$\langle f.L;\, C|\prod_{\alpha=c,\,s}\frac{1}{\sqrt{\mathcal{C}_{\alpha}}}(\hat{S}_{\alpha})^{L_{\alpha,\,-1/2}}\,\hat{O}^{l}_{\mathcal{N},\,j}|GS\rangle = \Big[\prod_{\alpha=c,\,s}\frac{1}{\sqrt{\mathcal{C}_{\alpha}}}\Big]\,\langle f.L;\, C|\hat{\Theta}^{l}_{\mathcal{N},\,j}|GS\rangle,$$

$$\langle f.L;\, C|\prod_{\alpha=c,\,s}\frac{1}{\sqrt{\mathcal{C}_{\alpha}}}(\hat{S}_{\alpha})^{L_{\alpha,\,-1/2}}\,\hat{O}^{l}_{\mathcal{N}}(k)|GS\rangle = \Big[\prod_{\alpha=c,\,s}\frac{1}{\sqrt{\mathcal{C}_{\alpha}}}\Big]\,\langle f.L;\, C|\hat{\Theta}^{l}_{\mathcal{N},\,k}|GS\rangle; \quad l = \pm 1. \quad (26)$$

By suitable use of equation (25), it is straightforward to show that the operators $\hat{\Theta}^{l}_{\mathcal{N},\,j}$ and $\hat{\Theta}^{l}_{\mathcal{N},\,k}$ are given by the following commutators,

$$\hat{\Theta}^{l}_{\mathcal{N},\,j} = \Big[\prod_{\alpha=c,\,s}(\hat{S}_{\alpha})^{L_{\alpha,\,-1/2}},\,\hat{O}^{l}_{\mathcal{N},\,j}\Big],$$
$$\hat{\Theta}^{l}_{\mathcal{N},\,k} = \Big[\prod_{\alpha=c,\,s}(\hat{S}_{\alpha})^{L_{\alpha,\,-1/2}},\,\hat{O}^{l}_{\mathcal{N},\,k}\Big], \quad L_{c,\,-1/2} \ \text{ and/or } \ L_{s,\,-1/2} > 0; \quad l = \pm 1, \quad (27)$$

or by,

$$\hat{\Theta}^{l}_{\mathcal{N},\,j} = \hat{O}^{l}_{\mathcal{N},\,j}; \qquad \hat{\Theta}^{l}_{\mathcal{N},\,k} = \hat{O}^{l}_{\mathcal{N},\,k}, \quad L_{c,\,-1/2} = L_{s,\,-1/2} = 0; \quad l = \pm 1. \quad (28)$$

Thus,

$$B^{l}_{\mathcal{N}}(k,\,\omega) = \sum_{\{\Delta N_{\alpha\nu}\},\,\{L_{\alpha,\,-1/2}\}}\Big(\prod_{\alpha=c,\,s}\frac{1}{\mathcal{C}_{\alpha}}\Big) \times \sum_{f} N_a |\langle f.L;\, C|\,\hat{\Theta}^{l}_{\mathcal{N},\,0}|GS\rangle|^2 \times \delta\Big(\omega - \Delta E_{cphs}\Big)\,\delta_{k,\,\Delta k_{cphs}}; \quad l = \pm 1. \quad (29)$$

Note that when the operator $\hat{\Theta}^{l}_{\mathcal{N},\,0}$ is given by equation (28) one has that $|f.L;\, C\rangle = |f;\, C\rangle$ in equation (29). If the commutator $[\prod_{\alpha=c,\,s}(\hat{S}_{\alpha})^{L_{\alpha,\,-1/2}},\,\hat{O}^{l}_{\mathcal{N},\,j}]$ of equation (27) vanishes, then the excitation generated by application of the corresponding operator $\hat{O}^{l}_{\mathcal{N},\,j}$ onto the ground state has no overlap with the excited energy eigenstate (23).

Similarly to $\hat{O}^{l}_{\mathcal{N},\,j}$, the corresponding operator $\hat{\Theta}^{l}_{\mathcal{N},\,j}$ can be written as a $\mathcal{N}$-electron operator. Let the numbers $\mathcal{N}^{l}_{l_c,\,l_s}$ of equation (6) refer to the operator $\hat{O}^{l}_{\mathcal{N},\,j}$ of the spectral-function expression of equation (7). Then we call $\bar{\mathcal{N}}^{l}_{l_c,\,l_s}$ the corresponding electronic numbers of the operator $\hat{\Theta}^{l}_{\mathcal{N},\,j}$ of the spectral-function expression of equation (29). The values are such that $\mathcal{N} = \sum_{l_c,\,l_s=\pm 1}\bar{\mathcal{N}}^{l}_{l_c,\,l_s} = \sum_{l_c,\,l_s=\pm 1}\mathcal{N}^{l}_{l_c,\,l_s}$ and,

$$\sum_{l_s=\pm 1}\bar{\mathcal{N}}^{+1}_{\pm 1,\,l_s} = \sum_{l_s=\pm 1}\mathcal{N}^{l}_{\pm 1,\,l_s} \pm 2L_{c,\,-1/2};$$
$$\sum_{l_c,\,l_s=\pm 1}\delta_{l_c,\,\pm l_s}\,\bar{\mathcal{N}}^{l}_{l_c,\,l_s} = \sum_{l_c,\,l_s=\pm 1}\delta_{l_c,\,\pm l_s}\,\mathcal{N}^{l}_{l_c,\,l_s} \mp 2L_{s,\,-1/2}; \quad l = \pm 1. \quad (30)$$

These relations provide information about the numbers of electronic creation and annihilation operators of the $\mathcal{N}$-electron operator $\hat{\Theta}^{l}_{\mathcal{N},\,j}$ expression relative to the corresponding numbers of the $\hat{O}^{l}_{\mathcal{N},\,j}$ expression. While the

number of electronic creation (and annihilation) operators decreases (and increases) by $2L_{c,-1/2}$, the number of electronic spin-down creation and spin-up annihilation (and spin-down annihilation and spin-up creation) operators decreases (and increases) by $2L_{s,-1/2}$.

We note that the numbers $\mathcal{N}^l_{l_c,l_s}$ of equation (6) for the operator $\hat{O}^l_{\mathcal{N},j}$ on the right-hand-side of equation (27) obey the sum rules (20). Thus, following the relations of equation (30), the numbers $\bar{\mathcal{N}}^l_{l_c,l_s}$ of the corresponding operator $\hat{\Theta}^l_{\mathcal{N},j}$ are such that,

$$\begin{aligned}\Delta L_c = 2\Delta S_c &= -\Delta N + 2L_{c,-1/2} = \sum_{l_c,l_s=\pm 1}(l_c)\,\bar{\mathcal{N}}^l_{l_c,l_s};\\ \Delta L_s = 2\Delta S_s &= \Delta(N_\uparrow - N_\downarrow) + 2L_{s,-1/2}\\ &= -\sum_{l_c,l_s=\pm 1}(l_c\,l_s)\,\bar{\mathcal{N}}^l_{l_c,l_s}. \end{aligned} \quad (31)$$

The first relation of equation (20) just states that the difference in the number of electronic creation and annihilation operators of the original $\mathcal{N}$-electron operator $\hat{O}^l_{\mathcal{N},j}$ equals the value ΔN of the electron number deviation generated by such an operator. Similarly, the first relation of equation (31) states that the difference in the number of rotated-electron annihilation and creation operators of $\hat{\Theta}^l_{\mathcal{N},j}$ equals twice the value $\Delta S_c = \Delta\eta$ of the η-spin value deviation generated by that $\mathcal{N}$-rotated-electron operator. Similar considerations apply to the second relations of equations (20) and (31).

We emphasize that all matrix elements of the general spectral-function expression (29) refer to regular energy eigenstates. Indeed, by changing from the spectral function representation (7) to (29) we have eliminated the explicit presence of $-1/2$ Yang holons and $-1/2$ HL spinons. This was done by evaluation of the contribution of these quantum objects to the $\mathcal{N}$-electron spectral weight. Such a procedure corresponds to the computation of the commutator $[\prod_{\alpha=c,s}(\hat{S}_\alpha)^{L_{\alpha,-1/2}},\,\hat{O}^l_{\mathcal{N},j}]$ on the right-hand side of equation (27).

Our next step is the expression of the operator $\hat{\Theta}^l_{\mathcal{N},j}$ for the general spectral-function expression (29) in terms of rotated-electron creation and annihilation operators. Here we use the results of references [3,9,20] concerning the expression of the rotated electrons in terms of $\pm 1/2$ holons, $\pm 1/2$ spinons, and $c0$ pseudofermions. It is this direct relation that makes convenient the rotated-electron expression for the $\mathcal{N}$-electron spectral functions. The expression of the local $\mathcal{N}$-electron operator $\hat{\Theta}^l_{\mathcal{N},j}$ in terms of rotated-electron creation and annihilation operators is obtained by use of the following relation,

$$\begin{aligned}\hat{\Theta}^l_{\mathcal{N},j} = e^{\hat{S}}\,\tilde{\Theta}^l_{\mathcal{N}_0,j}\,e^{-\hat{S}} &= \tilde{\Theta}^l_{\mathcal{N}_0,j} + \sum_{i=1}^{\infty}\sqrt{c^l_i}\,\tilde{\Theta}^l_{\mathcal{N}_i,j};\\ j = 1,2,...,N_a; \quad l &= \pm 1. \end{aligned} \quad (32)$$

Here $\hat{S}$ is the operator defined by equations (21)–(23) of reference [9] and $\tilde{\Theta}^l_{\mathcal{N}_0,j}$ has the same expression in terms of rotated-electron creation and annihilation operators as $\hat{\Theta}^l_{\mathcal{N},j}$ in terms of electronic creation and annihilation operators and thus $\mathcal{N}_0 = \mathcal{N}$. It is given by,

$$\begin{aligned}\tilde{\Theta}^l_{\mathcal{N}_0,j} = \hat{V}^\dagger(U/t)\,\hat{\Theta}^l_{\mathcal{N},j}\,\hat{V}(U/t) &= e^{-\hat{S}}\,\hat{\Theta}^l_{\mathcal{N},j}\,e^{\hat{S}};\\ j = 1,2,...,N_a; \quad l &= \pm 1. \end{aligned}$$

The operators $\tilde{\Theta}^l_{\mathcal{N}_i,j}$ on the right-hand side of equation (32) such that $i = 1,2,...$ can be written as a product of $\mathcal{N}_i$ rotated-electron creation and annihilation operators and the value of the coefficient c^l_i is a function of n, m, and U/t such that $c^l_i \to 0$ as $U/t \to \infty$. For instance, for $i = 1$ and $i = 2$ we find,

$$\sqrt{c^l_1}\,\tilde{\Theta}^l_{\mathcal{N}_1,j} = [\hat{S},\,\tilde{\Theta}^l_{\mathcal{N}_0,j}]; \quad j = 1,2,...,N_a; \quad l = \pm 1, \quad (33)$$

and

$$\begin{aligned}\sqrt{c^l_2}\,\tilde{\Theta}^l_{\mathcal{N}_2,j} = \frac{1}{2}\,[\hat{S},\,[\hat{S},\,\tilde{\Theta}^l_{\mathcal{N}_0,j}]];\ j = 1,2,...,N_a;\\ l = \pm 1, \end{aligned} \quad (34)$$

respectively, and the $i > 2$ operator terms are easily generated and involve similar commutators. For simplicity, here we omit the longer expressions of the latter terms.

It is useful for the study of the spectral-function expressions to divide each CPHS ensemble subspace in a set of well-defined subspaces. The number deviation $\Delta N_{\alpha\nu}$ for the $\alpha\nu = c0,\,s1$ branches and the number $N_{\alpha\nu} = \Delta N_{\alpha\nu}$ for the $\alpha\nu \neq c0,\,s1$ branches can be expressed in terms of other related numbers as follows,

$$\begin{aligned}\Delta N_{\alpha\nu} &= \Delta N^F_{\alpha\nu} + \Delta N^{NF}_{\alpha\nu};\\ \Delta N^F_{\alpha\nu} &= \Delta N^F_{\alpha\nu,+1} + \Delta N^F_{\alpha\nu,-1};\\ 2\Delta J^F_{\alpha\nu} &= \Delta N^F_{\alpha\nu,+1} - \Delta N^F_{\alpha\nu,-1};\\ \Delta N^F_{\alpha\nu,\iota} &= \Delta N^{0,F}_{\alpha\nu,\iota} + \iota\,Q^0_{\alpha\nu}/2\pi;\\ \Delta N^{0,F}_{\alpha\nu} &= \Delta N^{0,F}_{\alpha\nu,+1} + \Delta N^{0,F}_{\alpha\nu,-1} = \Delta N^F_{\alpha\nu};\\ \alpha\nu &= c0,\,s1 \quad \iota = \pm 1;\\ N_{\alpha\nu} &= N^F_{\alpha\nu} + N^{NF}_{\alpha\nu};\\ N^F_{\alpha\nu} &= N^F_{\alpha\nu,+1} + N^F_{\alpha\nu,-1};\\ 2J^F_{\alpha\nu} &= N^F_{\alpha\nu,+1} - N^F_{\alpha\nu,-1};\\ \alpha\nu &\neq c0,\,s1. \end{aligned} \quad (35)$$

Here $\Delta N^F_{\alpha\nu,\pm 1}$ is the deviation in the number of $\alpha\nu = c0,\,s1$ pseudofermions at the right $(+1)$ and left right (-1) *Fermi points*, $\Delta N^F_{\alpha\nu}$ and $\Delta J^F_{\alpha\nu}$ are the corresponding number and current number deviations, respectively, and $\Delta N^{NF}_{\alpha\nu}$ gives the deviation in the number of $\alpha\nu = c0,\,s1$ pseudofermions away from these points. Moreover, $\Delta N^{0,F}_{\alpha\nu,\pm 1}$ is the actual number of $\alpha\nu$ pseudofermions created or annihilated at the right $(+1)$ and left right (-1) *Fermi points* and $Q^0_{\alpha\nu}/2$ is the scatter-less phase shift on the right-hand side of equation (11). For the

$\alpha\nu \neq c0,\, s1$ branches, $N^F_{\alpha\nu,\,\iota}$ is the number of $\alpha\nu$ pseudofermions with limiting bare-momentum value $q = \iota\, q^0_{\alpha\nu}$ such that $\iota = \pm 1$, $J^F_{\alpha\nu}$ is the corresponding current number, and $N^{NF}_{\alpha\nu}$ is the number of $\alpha\nu$ pseudofermions whose bare-momentum values obey the inequality $|q| < q^0_{\alpha\nu}$.

Let us also consider the number $N^{phNF}_{\alpha\nu}$ of finite-momentum and finite-energy $\alpha\nu$ pseudofermion particle-hole processes (A), which refers to the $\alpha\nu = c0,\, s1$ branches only [3]. $N^{phNF}_{\alpha\nu}$ is zero or a positive integer such that $N^{phNF}_{\alpha\nu} = [\mathcal{N}_{\alpha\nu} - |\Delta N^{NF}_{\alpha\nu}|]/2$. Here $\mathcal{N}_{\alpha\nu}$ gives the number of $\alpha\nu$ pseudofermion creation and annihilation operators involved in the expression of the generators of the elementary processes (A).

The *J-CPHS ensemble subspaces* are the subspaces of a CPHS ensemble subspace spanned by the excited energy eigenstates with the same values for the numbers N^{phNF}_{c0}, N^{phNF}_{s1}, $\Delta N^F_{c0,\,+1}$, $\Delta N^F_{c0,\,-1}$, $\Delta N^F_{s1,\,+1}$, $\Delta N^F_{s1,\,-1}$, and sets of numbers $\{N^F_{\alpha\nu,\,+1}\}$ and $\{N^F_{\alpha\nu,\,-1}\}$ for the $\alpha\nu \neq c0,\, s1$ branches with finite pseudofermion occupancy in the CPHS ensemble subspace.

Use of equation (32) for $j = 0$ in the general spectral-function expression (29) leads to,

$$B^l_{\mathcal{N}}(k,\,\omega) = \sum_{i=0}^{\infty} c^l_i \sum_{\{\Delta N_{\alpha\nu}\},\{L_{\alpha,\,-1/2}\}} \Big[\sum_{\{N^{phNF}_{\alpha\nu}\},\{\Delta N^F_{\alpha\nu,\iota}\},\{N^F_{\alpha\nu,\iota}\}} B^{l,i}(k,\omega) \Big]; \quad c^l_0 = 1, \quad l = \pm 1, \quad (36)$$

where the summations $\sum_{\{\Delta N_{\alpha\nu}\},\{L_{\alpha,\,-1/2}\}}$ and $\sum_{\{N^{phNF}_{\alpha\nu}\},\{\Delta N^F_{\alpha\nu,\,\iota}\},\{N^F_{\alpha\nu,\,\iota}\}}$ run over CPHS ensemble subspaces and the corresponding J-CPHS ensemble subspaces of each of these spaces, respectively. The function $B^{l,i}(k,\,\omega)$ on the right-hand side of equation (36) reads,

$$B^{l,i}(k,\,\omega) = \Big(\prod_{\alpha=c,\,s} \frac{1}{\mathcal{C}_\alpha} \Big) \sum_f N_a |\langle f.L;\, JC|\, \tilde{\Theta}^l_{\mathcal{N}_i,\,0} |GS\rangle|^2 \times \delta\Big(\omega - l\Delta E_{j-cphs}\Big)\, \delta_{k,\,l\Delta k_{j-cphs}}; \quad l = \pm 1; \quad i = 0,1,2,..., \quad (37)$$

where the summation $\sum_f$ runs over the excited energy eigenstates $|f.L;\, JC\rangle$ which span each J-CPHS ensemble subspace. Thus, there is a function $B^{l,i}(k,\,\omega)$ for each of these subspaces. (We recall that $|f.L;\, JC\rangle$ is the LWS of a state $|f;\, JC\rangle$ related to it by the general Eq. (23).)

Finally, let us use a notation for the number of spin-down and spin-up rotated-electron creation and annihilation operators of the operator $\tilde{\Theta}^l_{\mathcal{N}_i,\,j}$ such that $i = 0,1,2,...$ similar to that associated with the numbers $\bar{\mathcal{N}}^l_{l_c,\,l_s}$ of equation (30). Thus, we introduce the numbers,

$$\mathcal{N}_i = \sum_{l_c,\,l_s=\pm 1} \bar{\mathcal{N}}^{l,i}_{l_c,\,l_s}; \quad l = \pm 1; \quad i = 0,1,2..., \quad (38)$$

which refer to the operator $\tilde{\Theta}^l_{\mathcal{N}_i,\,j}$. Here $\bar{\mathcal{N}}^{l,i}_{l_c,\,l_s}$ is the number of rotated-electron creation and annihilation operators for $l_c = -1$ and $l_c = +1$, respectively, and with spin down and spin up for $l_s = -1$ and $l_s = +1$, respectively. The operator $\tilde{\Theta}^l_{\mathcal{N}_0,\,j}$ of equation (32) has the same four rotated-electron numbers $\{\bar{\mathcal{N}}^{0,l}_{l_c,\,l_s}\} = \{\bar{\mathcal{N}}^l_{l_c,\,l_s}\}$ as the corresponding operator $\hat{\Theta}^l_{\mathcal{N},\,j}$ in terms of electrons.

4 Rotated-electron sum rules, selection rules, and elementary processes in terms of pseudofermion operators

In this section we provide sum rules and selection rules which for the PS arise from the direct relation between rotated electrons and the holons, spinons, and pseudofermions. Furthermore, we use such a relation to express the elementary rotated-electron processes in terms of the pseudofermion creation and annihilation operators.

An important symmetry is that all six generators of the η-spin and spin $SU(2)$ algebras are invariant under the electron–rotated-electron unitary transformation [9]. Thus, the number of spin-projection σ electrons equals the number of spin-projection σ rotated electrons. This also applies to the deviations ΔS_c and ΔS_s in the η-spin and spin values, respectively, generated by application onto the ground state of a $\mathcal{N}$-electron operator. This symmetry implies that all $i = 0,1,2,...$ operators $\tilde{\Theta}^l_{\mathcal{N}_i,\,j}$ on the right-hand side of equation (32) generate the same deviations ΔS_c and ΔS_s, as the operator $\hat{\Theta}^l_{\mathcal{N},\,j}$ on the left-hand side of the same equation. It follows that the values $\bar{\mathcal{N}}^{l,i}_{l_c,\,l_s}$ for all these $i = 0,1,2,...$ operators with the same value of $l = \pm 1$ obey the following sum rules,

$$\Delta L_c = 2\Delta S_c = -\Delta N + 2L_{c,\,-1/2} = \sum_{l_c,\,l_s=\pm 1} (l_c)\, \bar{\mathcal{N}}^{l,i}_{l_c,\,l_s};$$
$$\Delta L_s = 2\Delta S_s = \Delta(N_\uparrow - N_\downarrow) + 2L_{s,\,-1/2} = -\sum_{l_c,\,l_s=\pm 1} (l_c\, l_s)\, \bar{\mathcal{N}}^{l,i}_{l_c,\,l_s}; \quad l = \pm 1; \quad i = 0,1,2,... \quad (39)$$

These rules provide useful information about the expression of all $i = 1,2,...$ operators $\tilde{\Theta}^l_{\mathcal{N}_i,\,j}$. In addition to the rotated-electron creation and annihilation operators of $\tilde{\Theta}^l_{\mathcal{N}_0,\,j}$, such an expression includes pairs of rotated-electron creation and annihilation operators with the same spin projection σ. Thus, such additional creation and annihilation operators only generate rotated-electron particle-hole excitations and do not change the net number of spin-projection σ rotated electrons created or annihilated by application of the operators $\tilde{\Theta}^l_{\mathcal{N}_i,\,j}$ onto the ground state. The general situation refers to $\mathcal{N}$-electron operators that are not invariant under the electron - rotated-electron unitary transformation. (The problem is trivial for those that are invariant, once $\tilde{\Theta}^l_{\mathcal{N}_i,\,j} = 0$ for $i > 0$ in that case.) The precise form of $\tilde{\Theta}^l_{\mathcal{N}_i,\,j}$ for $i = 1,2,...$ depends on the specific $\mathcal{N}$-electron operator under consideration. However, a general property that follows from the relations (39) is that for increasing values of $i = 1,2,...$ the operators $\tilde{\Theta}^l_{\mathcal{N}_i,\,j}$

are constructed by adding to $\tilde{\Theta}^{l}_{\mathcal{N}_0,\,j}$ an increasing number of *particle-hole* elementary spin-projection σ rotated-electron pairs.

In equation (32) the $\mathcal{N}$-electron operator $\hat{\Theta}^{l}_{\mathcal{N},\,j}$ is expressed in terms of rotated-electron creation and annihilation operators. From the direct relation between the rotated electrons and the holons, spinons, and pseudofermions it is straightforward to find useful selection rules. Such rules refer to restrictions in the values of the number of $-1/2$ holons and thus of 2ν-holon composite $c\nu$ pseudofermions generated by application onto the ground state of each of the $i = 0, 1, 2, ...$ operators $\tilde{\Theta}^{l}_{\mathcal{N}_i,\,j}$ of expression (32). [The expression of these operators determines the value of the $\mathcal{N}$-electron spectral function of Eq. (36), as confirmed by the form of the related functions (37).] For the PS excited energy eigenstates which have finite overlap with the $\mathcal{N}$-electron excitations, the values of the $-1/2$-holon number, $M_{c,\,-1/2}$, and number of finite-energy and finite-momentum $c0$ pseudofermion particle-hole processes, N^{phNF}_{c0}, of the elementary processes (A) [3] are restricted to the following ranges,

$$M_{c,\,-1/2} = L_{c,\,-1/2} + \sum_{\nu=1}^{\infty}\nu\,N_{c\nu} = 0, 1, ..., \sum_{l_s=\pm 1}\bar{\mathcal{N}}^{l,i}_{-1,\,l_s};$$
$$N^{phNF}_{c0} = 0, 1, ..., \min\left\{\sum_{l_s=\pm 1}\bar{\mathcal{N}}^{l,i}_{-1,\,l_s}, \sum_{l_s=\pm 1}\bar{\mathcal{N}}^{l,i}_{+1,\,l_s}\right\};$$
$$i = 0, 1, 2, ... \quad (40)$$

Here the numbers $\bar{\mathcal{N}}^{l,i}_{l_c,\,l_s}$ are those of equation (38) for the operator $\tilde{\Theta}^{l}_{\mathcal{N}_i,\,j}$. The $i = 0$ operator $\tilde{\Theta}^{l}_{\mathcal{N}_0,\,j}$ has the same expression in terms of rotated-electron creation and annihilation operators as the corresponding operator $\hat{\Theta}^{l}_{\mathcal{N},\,j}$ of equation (32) in terms of electronic creation and annihilation operators. Therefore, for $i = 0$ the selection rules given in equation (40) read,

$$M_{c,\,-1/2} = L_{c,\,-1/2} + \sum_{\nu=1}^{\infty}\nu\,N_{c\nu} = 0, 1, ..., \sum_{l_s=\pm 1}\bar{\mathcal{N}}^{l}_{-1,\,l_s};$$
$$N^{phNF}_{c0} = 0, 1, ..., \min\left\{\sum_{l_s=\pm 1}\bar{\mathcal{N}}^{l}_{-1,\,l_s}, \sum_{l_s=\pm 1}\bar{\mathcal{N}}^{l}_{+1,l_s}\right\}, \quad (41)$$

where the numbers $\bar{\mathcal{N}}^{l}_{-1,\,l_s} = \bar{\mathcal{N}}^{l,0}_{-1,\,l_s}$ are those of equation (30) specific to the operator $\hat{\Theta}^{l}_{\mathcal{N},\,j}$.

The first exact ground-state charge selection rule of equation (40) concerning the number of $-1/2$ holons, $M_{c,\,-1/2}$, is equivalent to the following selection rule involving the number deviation $-\Delta M_c = \Delta M_s = \Delta N_{c0}$,

$$\sum_{l_c,\,l_s=\pm 1}(l_c)\,\bar{\mathcal{N}}^{l,i}_{l_c,\,l_s} \leq \Delta M_c \leq \mathcal{N}_i;$$
$$-\ \mathcal{N}_i \leq \Delta N_{c0} = \Delta M_s \leq -\sum_{l_c,\,l_s=\pm 1}(l_c)\,\bar{\mathcal{N}}^{l,i}_{l_c,\,l_s};$$
$$i\ =\ 0, 1, 2, ... \quad (42)$$

Indeed, the combination of the inequalities (42) with the relations (27)-(29) of reference [9] and that of equation (39), readily confirms the equivalence of the first selection rule given in equation (40) and that of equation (42).

Moreover, the $-1/2$ spinon number deviation $\Delta M_{s,\,-1/2}$ is fully determined by the value of the $-1/2$ holon number of the first selection rule of equation (40) and reads,

$$\Delta M_{s,\,-1/2} = L_{s,\,-1/2} + \Delta N_{s1} + \sum_{\nu=2}^{\infty}\nu\,N_{s\nu}$$
$$= \Delta N_{\downarrow} - M_{c,\,-1/2}. \quad (43)$$

Equations (18), (19), (39), and (43) define sum rules obeyed by the values of the deviations in the quantum-object numbers and equations (21), (40), and (42) correspond to selection rules for the permitted values of these deviations. Such sum rules and selection rules define the set of CPHS ensemble subspaces which contain the excited energy eigenstates with finite overlap with the $\mathcal{N}$-electron excitations under consideration.

While the above rules are exact, direct evaluation of the weights by the method introduced in Section 5 and further developed in reference [3] reveals that 94% to 98% of the $\mathcal{N}$-electron weight corresponds to excited energy eigenstates with numbers in the following range,

$$L_{s,\,-1/2} + \sum_{\nu=1}^{\infty}(\nu-1)\,N_{s\nu} = 0, 1, 2, ..., \sum_{l_c,\,l_s=\pm 1}\delta_{l_c,\,l_s}\,\bar{\mathcal{N}}^{l,i}_{l_c,\,l_s};$$
$$i = 0, 1, 2, ... \quad (44)$$

For $i = 0$ the relation (44) can be written as,

$$L_{s,\,-1/2} + \sum_{\nu=1}^{\infty}(\nu-1)\,N_{s\nu} = 0, 1, 2, ..., \sum_{l_c,\,l_s=\pm 1}\delta_{l_c,\,l_s}\,\bar{\mathcal{N}}^{l}_{l_c,\,l_s}, \quad (45)$$

where the numbers $\bar{\mathcal{N}}^{l}_{l_c,\,l_s} = \bar{\mathcal{N}}^{l,0}_{l_c,\,l_s}$ are those of equation (30) specific for the operator $\hat{\Theta}^{l}_{\mathcal{N},\,j}$ of equation (32).

Local $-1/2$ holons (and $-1/2$ spinons) correspond to local 2ν-holon composite $c\nu$ pseudofermions (and 2ν-spinon composite $s\nu$ pseudofermions). Local $\alpha\nu$ pseudofermions are associated with the operators $f^{\dagger}_{x_j,\,\alpha\nu}$ and $f_{x_j,\,\alpha\nu}$ on the right-hand side of equation (34) of reference [3]. Let us denote the rotated-electron spin projections $\sigma = \uparrow, \downarrow$ by $\sigma = -1/2, +1/2$, respectively, and consider the elementary processes of the $\mathcal{N}$-electron excitations in terms of occupancy configurations of local $\pm 1/2$ holons, $\pm 1/2$ spinons, and $c0$ pseudofermions:

(i) to create one spin-projection $\sigma = \pm 1/2$ rotated electron at the unoccupied site j, we need to annihilate a local $+1/2$ holon and create a local $c0$ pseudofermion and a local $\pm 1/2$ spinon at the same site. Annihilation of a spin-projection $\sigma = \pm 1/2$ rotated electron at a spin-projection $\sigma = \pm 1/2$ rotated-electron singly occupied site j, involves the opposite processes;

(ii) to create one spin-projection $\sigma = \pm 1/2$ rotated electron at a spin-projection $\sigma = \mp 1/2$ rotated-electron singly occupied site j, we need to annihilate a local $\mp 1/2$ spinon and a local $c0$ pseudofermion and to create a local $-1/2$ holon at such a site. Again, to annihilate a spin-projection $\sigma = \pm 1/2$ rotated electron at a rotated-electron doubly occupied site j, involves the opposite processes;

(iii) the creation of two rotated electrons of opposite spin projection onto the unoccupied site j involves the annihilation of a local $+1/2$ holon and the creation of a local $-1/2$ holon at such a site. Annihilation of two rotated electrons of opposite spin projection onto the doubly-occupied site j, involves the opposite processes;

(iv) the annihilation of one spin-projection $\sigma = \pm 1/2$ rotated electron and creation of one spin-projection $\sigma = \mp 1/2$ rotated electron at the singly-occupied site j, involves the annihilation of one local $\pm 1/2$ spinon and the creation of one local $\mp 1/2$ spinon.

Other processes can be expressed as suitable combinations of the above elementary processes. The local rotated-electron operator terms which transfer spectral weight from the ground state to each of the J-CPHS ensemble subspaces appearing in the state summation of the spectral-function expression (36) have a specific and uniquely defined form in terms of $c0$ pseudofermion and composite $\alpha\nu$ pseudofermion creation and annihilation operators. In order to find the pseudofermion form of these operator terms it is crucial to take into account the initial ground-state pseudofermion occupancies, given in equations (C.24, C.25) of reference [9]. (We recall that the pseudoparticle-number values of the latter equations equal those of the corresponding pseudofermion numbers.)

Before illustrating how the elementary processes (i)–(iv) are generated by the pseudofermion creation and annihilation operators, it is convenient to provide some basic rules for the use of the latter operators. Since following the use of the relations of equation (26) all matrix elements are between the ground state and regular excited states, in the processes considered below, the deviations in the numbers of Yang holons ($\alpha = c$) and HL spinons ($\alpha = s$) are such that $\Delta L_\alpha = \Delta L_{\alpha,+1/2}$. Some of these processes involve creation or annihilation of $+1/2$ Yang holons and/or $+1/2$ HL spinons. However, we recall that within the pseudofermion representation, the $+1/2$ Yang holons and $+1/2$ HL spinons do not appear explicitly. Such processes are taken into account by the deviations in the number of discrete bare-momentum (and canonical-momentum) values and effective $\alpha\nu$ lattice sites of the $c\nu \neq c0$ branches and/or $s\nu$ branches, respectively. Given the values of the corresponding pseudofermion number deviations, this is readily confirmed if one compares the number (B.6) of reference [9] of discrete bare-momentum values and of effective lattice sites of the excited energy eigenstate and ground state CPHS ensemble subspaces. Since $\Delta L_\alpha = \Delta L_{\alpha,+1/2}$, note that following equations (B.6) and (B.7) of reference [9], the value of the number $N^*_{\alpha\nu}$ changes when the value of the number $L_c = L_{c,+1/2}$ of $+1/2$ Yang holons and/or $L_s = L_{s,+1/2}$ of $+1/2$ HL spinons also changes. Thus, creation and annihilation of $+1/2$ Yang holons (and $+1/2$ HL spinons) are processes that are taken into account in the definition of the effective $c\nu \neq c0$ pseudofermion lattices of the initial ground state and excited energy eigenstates.

In the following we provide different examples of local rotated-electron operator expressions in terms of pseudofermion creation and annihilation operators. For simplicity, each of such pseudofermion expressions corresponds to the term of the local rotated-electron operator which transfers spectral weight from the initial ground state onto a single excitation J-CPHS ensemble subspace. Such a pseudofermion term includes a coefficient factor $1/C_J$ whose value is well defined for each subspace. The full local rotated-electron operator term which transfers spectral weight from the ground state to a given J-CPHS ensemble subspace is the product of that studied here by another pseudofermion operator term given in the ensuing section. The latter operator transfers from the ground state to the J-CPHS ensemble subspace the part of the spectral weight which corresponds to the processes (B) and (C), whereas the pseudofermion terms studied here transfer the part of that weight associated with the processes (A).

A $i = 0$ local rotated-electron operator $\tilde{\Theta}^l_{\mathcal{N}_0,j}$ always has one or a few *dominant* CPHS ensemble subspaces which correspond to the whole spectral weight transferred from the ground state in well defined limits. For one-electron problems such that $\mathcal{N}_0 = \mathcal{N} = 1$ this refers to the limits where the spectral-weight distribution is δ-function like, as in equation (77) of reference [3]. For $\mathcal{N}_0 = \mathcal{N} = 2$, to the limits where such a distribution can be expressed as a simple integral whose integrand is a δ function, as in equation (78) of the same reference. In the general $\mathcal{N}_0 = \mathcal{N} > 2$ case, to the limits where the spectral-weight distribution can be written as an integral whose integrand is a product of $[\mathcal{N}-1]$ δ functions. For instance, for $\mathcal{N} = 1$ this occurs for $U/t \rightarrow 0$. For the one-electron problem the amount of spectral weight transferred from the ground state to the set of J-CPHS ensemble subspaces contained in the dominant CPHS ensemble subspaces is weakly dependent on U/t: while for $U/t \ll 1$ it corresponds to the whole spectral weight transferred from the ground state by the local rotated-electron operator, for $U/t \gg 1$ it corresponds typically to more than 0.94% of that weight. (Comparison of the amount of transferred weight for $U/t \ll 1$ with that obtained by use of the methods of Ref. [16] for $U/t \gg 1$ confirms such a weak U/t dependence.) For U/t finite there arise an infinite number of pseudofermion terms, each corresponding to a J-CPHS ensemble subspace compatible with the local rotated-electron operator. Another example is the $\mathcal{N} = 2$ charge dynamical structure factor, where there are different dominant CPHS ensemble subspaces for $U/t \rightarrow 0$ and $U/t \rightarrow \infty$, respectively. In this case the amount of spectral weight transferred from the ground state to the set of J-CPHS ensemble subspaces contained in the dominant CPHS ensemble subspaces is a decreasing (and increasing) function of U/t for the $U/t \rightarrow 0$ (and $U/t \rightarrow \infty$) dominant subspaces and vanishes as $U/t \rightarrow \infty$ (and

$U/t \rightarrow 0$). Again, for intermediate finite values of U/t there arise an infinite number of pseudofermion terms, each corresponding to a J-CPHS ensemble subspace compatible with the local rotated-electron operator. However, for all $i = 0$ local rotated-electron operators $\tilde{\Theta}^{l}_{\mathcal{N}_0,\,j}$ the pseudofermion terms associated with the dominant subspaces together with a small number of other terms correspond to more than 99% of the spectral weight. It follows that in applications of the pseudofermion dynamical theory introduced here and in reference [3] only a finite number of pseudofermion terms should be considered.

The $\alpha\nu = c0,\, s1$ pseudofermion number deviations and $\alpha\nu \neq c0,\, s1$ pseudofermion numbers are related to the rotated-electron number deviations by equations (18) and (19). Given the values of the $\alpha\nu = c0,\, s1$ pseudofermion number deviations and $\alpha\nu \neq c0,\, s1$ pseudofermion numbers of the specific J-CPHS ensemble subspace under consideration, the expression of the local rotated-electron operator in terms of pseudofermion creation and annihilation operators is always uniquely defined. Let us start by providing some of the simplest pseudofermion operator terms of local rotated-electron operators. For local one- and two-rotated-electron operators these operator terms involve in general $\alpha\nu$ pseudofermion creation and/or annihilation operators belonging to branches such that $\nu < 2$. The case of other terms associated with excitation J-CPHS ensemble subspaces generated from the ground state by processes involving creation of composite $\alpha\nu$ pseudofermions for $\nu > 1$ is discussed later.

In the following expressions the $\alpha\nu$ effective lattice integer site index j' is such that $j' = 1, 2, ..., N^{*}_{\alpha\nu}$. An important property is that an operator whose expression in terms of rotated-electron operators is local at $x_j = ja = j$ can be written as a product of local $\alpha\nu$ pseudofermion operators at $x_{j'} \approx x_j$ where $x_{j'} = j' a^{0}_{\alpha\nu}$. Here and in all expressions given below j' is defined for the $\alpha\nu \neq c0$ branches as the closest integer number to $jn^{*}_{\alpha\nu}$, whereas $j' = j$ for $\alpha\nu = c0$. We note that for the former branches the site j' occupied by one $\alpha\nu$ pseudofermion corresponds to 2ν sites of the rotated-electron lattice. Thus, $|x_{j'} - x_j|$ is always smaller than the very small intrinsic uncertainty which corresponds to the 2ν rotated-electron lattice sites occupied by the local $\alpha\nu$ pseudofermion. Moreover, we emphasize that the rotated-electron lattice site j associated with the effective $\alpha\nu \neq c0$ lattice site $j' \approx jn^{*}_{\alpha\nu}$ defined above always belongs to the domain of 2ν rotated-electron lattice sites of j'. Here and below we use the equality $j' = jn^{*}_{\alpha\nu}$ to denote the integer number j' defined above. Thus, the site j' is such that $j' = j$ for $\alpha\nu = c0$ operators, $j' = jn_{\uparrow}$ for $\alpha\nu = s1$ operators, $j' = j[1-n]$ for $c\nu \neq c0$ operators when $n < 1$, and $j' = j[n_{\uparrow} - n_{\downarrow}]$ for $s\nu \neq s1$ operators when $m > 0$. The following local rotated-electron operator expressions in terms of pseudofermions, whose coefficient C_J is different for each operator, refer to the elementary processes (A) subspace:

(i) One of the simplest processes for creation of one spin-down rotated electron at the unoccupied site j involves the creation of a local $c0$ pseudofermion with the operator $f^{\dagger}_{x_j,\,c0}$ and of a local $s1$ pseudofermion with the operator $f^{\dagger}_{x_{j'},\,s1}$ such that $j' = jn_{\uparrow}$,

$$\begin{aligned}
\tilde{c}^{\dagger}_{j,\downarrow}\,(1-\tilde{n}_{j,\uparrow}) &= \frac{1}{C_J}\, f^{\dagger}_{x_{j'},\,s1}\, f^{\dagger}_{x_j,\,c0}; \\
C_J &= e^{i\,j\Delta P_J}\,\frac{G_C}{G_J}; \\
G_J &= \prod_{\alpha\nu}\Big[\theta(\mathcal{N}_{\alpha\nu})(n^{*}_{\alpha\nu})^{\frac{\mathcal{N}_{\alpha\nu}-1}{2}} + [1-\theta(\mathcal{N}_{\alpha\nu})]\Big], \\
\mathcal{N}_{\alpha\nu} &= |\Delta N^{NF}_{\alpha\nu}| + 2N^{phNF}_{\alpha\nu}, \quad \alpha\nu = c0,\, s1; \\
\mathcal{N}_{\alpha\nu} &= N^{NF}_{\alpha\nu}, \quad \alpha\nu \neq c0,\, s1,
\end{aligned} \tag{46}$$

and thus $\tilde{c}_{j,\downarrow}\,(1-\tilde{n}_{j,\uparrow}) = \frac{1}{C_J}\, f_{x_j,\,c0}\, f_{x_{j'},\,s1}$ refers to annihilation of one spin-down rotated electron at the singly-occupied site j. In equation (46), $\tilde{n}_{j,\sigma} = \tilde{c}^{\dagger}_{j,\sigma}\,\tilde{c}_{j,\sigma}$ is the local spin-projection σ rotated-electron density operator.

Note that the only j dependence of the coefficient C_J whose general expression is provided in equation (46) is through the phase factor $e^{i\,j\Delta P_J}$, and thus the real and positive number $|C_J|$ is independent of the spatial coordinate j. In the expression of the U/t independent real positive number G_J given in that equation, $\mathcal{N}_{\alpha\nu}$ equals the number of $\alpha\nu$ pseudofermion creation and annihilation operators of the expression of the operator under consideration. For instance, $\mathcal{N}_{c0} = \mathcal{N}_{s1} = 1$ for both the above operators $\frac{1}{C_J}\, f^{\dagger}_{x_{j'},\,s1}\, f^{\dagger}_{x_j,\,c0}$ and $\frac{1}{C_J}\, f_{x_j,\,c0}\, f_{x_{j'},\,s1}$. While the values of G_J and of the momentum deviation ΔP_J are specific to each excited J-CPHS ensemble subspace, that of the real positive constant G_C is fixed and well defined for each excited CPHS ensemble subspace. Application of the operator $\frac{1}{C_J}\, f^{\dagger}_{x_{j'},\,s1}\, f^{\dagger}_{x_j,\,c0}$ of equation (46) onto the initial ground state leads to an excitation spanned by excited energy eigenstates belonging to the same J-CPHS ensemble subspace. The actual value of C_J is thus that corresponding to such a subspace. The same applies to the coefficients C_J of the other operators given below. Note that $G_J = 1$ for the simple operator expressions given in equation (46) and below in equations (47)–(53). Importantly, for the dominant CPHS ensemble subspaces considered above G_C reads $G_C = 1$ for all values of U/t. It follows that in the pseudofermion expressions of the operator (46) and operators (47)–(51) given below the coefficient C_J reduces to a phase factor, $C_J = e^{i\,j\Delta P_J}$, and thus is such that $|C_J| = 1$. Moreover, for other $i = 0$ rotated-electron operators as those provided below in equations (52) and (53) the value of the coefficient G_C is independent of U/t. (The general expression of the momentum deviation ΔP_J is given in Section 5 and that of G_C is provided below in equation (68).) That for $\mathcal{N}$-electron operators such that $\mathcal{N} = 1, 2$ the spectral weight generated by application onto the ground state of the $i > 0$ rotated-electron operators corresponding to the $\sum_i$ summation of the last term on the right-hand side of equation (32) is extremely small and can be ignored is confirmed by the recent studies of reference [22].

To create one spin-up rotated electron at the empty site j, a simple process corresponds to create a local $c0$

pseudofermion with the operator $f^{\dagger}_{x_j,\,c0}$,

$$\tilde{c}^{\dagger}_{j,\uparrow}\,(1-\tilde{n}_{j,\downarrow}) = \frac{1}{C_J}\,f^{\dagger}_{x_j,\,c0}, \tag{47}$$

and $\tilde{c}_{j,\uparrow}\,(1-\tilde{n}_{j,\downarrow}) = \frac{1}{C_J}\,f_{x_j,\,c0}$ to annihilation of one spin-up rotated electron at the singly-occupied site j. Such processes also involve creation and annihilation, respectively, of an empty site in the effective $s1$ lattice. When the initial ground state belongs to a $m = 0$ CPHS ensemble subspace, there is for the former process a single $s1$ pseudofermion hole in the excited state, which corresponds to the created site.

We note that the processes of the operator expressions of equations (46) and (47) also involve the annihilation of a $+1/2$ Yang holon, whereas the processes of the operator expressions $\tilde{c}_{j,\downarrow}\,(1-\tilde{n}_{j,\uparrow}) = \frac{1}{C_J}\,f_{x_j,\,c0}\,f_{x_{j'},\,s1}$ and $\tilde{c}_{j,\uparrow}\,(1-\tilde{n}_{j,\downarrow}) = \frac{1}{C_J}\,f_{x_j,\,c0}$ involve the creation of a $+1/2$ Yang holon. Similarly, the processes of the operator expression of equation (47) and those of $\tilde{c}_{j,\uparrow}\,(1-\tilde{n}_{j,\downarrow}) = \frac{1}{C_J}\,f_{x_j,\,c0}$ involve the creation and annihilation, respectively, of a $+1/2$ HL spinon. In the remaining cases considered below we do not specify the elementary processes of creation or annihilation of $+1/2$ Yang holons and $+1/2$ HL spinons, which are taken into account implicitly by the pseudofermion description, as discussed above.

(ii) One of the simplest processes associated with the creation of one spin-up rotated electron at a spin-down rotated-electron singly occupied site j involves the annihilation a local $c0$ pseudofermion with the operator $f_{x_j,\,c0}$ and of a local $s1$ pseudofermion with the operator $f_{x_{j'},\,s1}$ and the creation of a local $c1$ pseudofermion with the operator $f^{\dagger}_{x_{j''},\,c1}$ such that $j' = jn_{\uparrow}$ and $j'' = j[1-n]$, respectively,

$$\tilde{c}^{\dagger}_{j,\uparrow}\,\tilde{n}_{j,\downarrow} = \frac{1}{C_J}\,f^{\dagger}_{x_{j''},\,c1}\,f_{x_j,\,c0}\,f_{x_{j'},\,s1}. \tag{48}$$

Then $\tilde{c}_{j,\uparrow}\,\tilde{n}_{j,\downarrow} = \frac{1}{C_J}\,f^{\dagger}_{x_{j'},\,s1}\,f^{\dagger}_{x_j,\,c0}\,f_{x_{j''},\,c1}$ refers to annihilation of one spin-up rotated electron at a doubly occupied site j. Moreover, to create one spin-down rotated electron at a spin-up rotated-electron singly occupied site j, a simple process corresponds to annihilate a local $c0$ pseudofermion with the operator $f_{x_j,\,c0}$ and to create a local $c1$ pseudofermion with the operator $f^{\dagger}_{x_{j'},\,c1}$ such that $j' = j[1-n]$,

$$\tilde{c}^{\dagger}_{j,\downarrow}\,\tilde{n}_{j,\uparrow} = \frac{1}{C_J}\,f^{\dagger}_{x_{j'},\,c1}\,f_{x_j,\,c0}. \tag{49}$$

In this case $\tilde{c}_{j,\downarrow}\,\tilde{n}_{j,\uparrow} = \frac{1}{C_J}\,f^{\dagger}_{x_j,\,c0}\,f_{x_{j'},\,c1}$ corresponds to annihilation of one spin-down rotated electron at a doubly occupied site j.

(iii) A simple process involved in the creation of two rotated electrons of opposite spin projection onto the empty site j corresponds to creation of a local $c1$ pseudofermion with the operator $f^{\dagger}_{x_{j'},\,c1}$ such that $j' = j[1-n]$,

$$\tilde{c}^{\dagger}_{j,\downarrow}\,\tilde{c}^{\dagger}_{j,\uparrow} = \frac{1}{C_J}\,f^{\dagger}_{x_{j'},\,c1}. \tag{50}$$

It follows that $\tilde{c}_{j,\uparrow}\,\tilde{c}_{j,\downarrow} = \frac{1}{C_J}\,f_{x_{j'},\,c1}$ refers to annihilation of two rotated electrons of opposite spin projection onto a doubly-occupied site j. This involves annihilation of a local $c1$ pseudofermion with the operator $f_{x_{j'},\,c1}$ such that $j' = j[1-n]$.

(iv) One of the simplest processes associated with the annihilation of one spin-up rotated electron and creation of one spin-down rotated electron at the singly-occupied site j, involves the creation of a local $s1$ pseudofermion with the operator $f^{\dagger}_{x_{j'},\,s1}$ such that $j' = jn_{\uparrow}$,

$$\tilde{c}^{\dagger}_{j,\downarrow}\,\tilde{c}_{j,\uparrow} = \frac{1}{C_J}\,f^{\dagger}_{x_{j'},\,s1}. \tag{51}$$

Then $\tilde{c}^{\dagger}_{j,\downarrow}\,\tilde{c}_{j,\uparrow} = \frac{1}{C_J}\,f_{x_{j'},\,s1}$ corresponds to annihilation of one spin-down rotated electron and creation of one spin-up rotated electron at the singly-occupied site j. This involves the annihilation of a local $s1$ pseudofermion with the operator $f_{x_{j'},\,s1}$ such that $j' = jn_{\uparrow}$.

For local rotated-electron operators generating more complex processes involving creation or annihilation of several rotated electrons, the creation and annihilation of local $c0$ pseudofermions is always associated with creation and annihilation of rotated-electron singly occupied sites, respectively. Since the local $c0$ pseudofermions and $c0$ pseudofermion holes occupy the same sites j_l and j_h as the rotated-electron singly occupied sites and rotated-electron doubly-occupied and unoccupied sites, respectively, there is a one-to-one correspondence between the rotated-electron and $c0$ pseudofermion algebras.

However, once the composite local $\alpha\nu \neq c0$ pseudofermions have internal structure that involves 2ν rotated-electron sites with different index j, the operational relation of rotated electrons to such composite quantum objects is more involved. This justifies why the expressions of the local rotated-electron operators in terms of creation and annihilation pseudofermion operators involve a superposition of different pseudofermion expressions, corresponding to the set of compatible J-CPHS ensemble subspaces. Nevertheless, creation onto the ground state of a $c\nu$ pseudofermion (and $s\nu$ pseudofermion) always involves ν rotated-electron doubly occupied sites and ν unoccupied sites (and ν spin-down rotated-electron singly occupied sites ν spin-up rotated-electron singly occupied sites). In general, the excited-energy-eigenstate ν rotated-electron unoccupied sites (and ν spin-up rotated-electron singly occupied sites) of a created $c\nu$ pseudofermion (and $s\nu$ pseudofermion) are generated by annihilating an equal number of $+1/2$ Yang holons (and $+1/2$ HL spinons) of the initial ground state.

For the creation of a local $c\nu$ pseudofermion, each of the ν new created rotated-electron doubly occupied sites can result from creation of a rotated-electron pair onto an unoccupied site or of a rotated electron onto a singly-occupied site. The latter case involves always one of the elementary processes associated with the pseudofermion terms given just after equations (46) and (47). On the

other hand, for the creation of a local $s\nu$ pseudofermion such that $\nu > 1$, the ν involved spin-down rotated-electron singly occupied sites can result from creation of spin-down rotated electrons onto unoccupied sites or from recombination of pre-existing ground-state $s1$ pseudofermions, as further discussed below.

For instance, let us consider two J-CPHS ensemble subspaces contained in different CPHS ensemble subspaces which except for the occupancies of the $c1$ and $c2$ branches have the same pseudofermion numbers. For such branches, one has $\{N_{c1} = 2,\, N_{c2} = 0\}$ for the J-CPHS ensemble subspace (I) and $\{N_{c1} = 0,\, N_{c2} = 1\}$ for the J-CPHS ensemble subspace (II). Let us consider that the local rotated-electron operator behind the transitions to both subspaces is the same and involves creation of two rotated electrons of spin projections $\sigma =\uparrow$ and $\sigma =\downarrow$ onto the spin-down singly occupied site j and spin-up singly occupied site $j+1$, respectively. For the subspace (I), this corresponds simply to the process of equation (48) for the site j and the process of equation (49) for the site $j+1$. For the subspace (II), in order to create two rotated electrons of spin projections $\sigma =\uparrow$ and $\sigma =\downarrow$ onto the spin-down singly occupied site j and spin-up singly occupied site $j+1$, respectively, we need to annihilate two local $c0$ pseudofermions with the operators $f_{x_j,\,c0}$ and $f_{x_{j+1},\,c0}$ and a local $s1$ pseudofermion with the operator $f_{x_{j'},\,s1}$ such that $j' = jn_\uparrow$ and to create a local $c2$ pseudofermion with the operator $f^\dagger_{x_{j''},\,c2}$ such that $j'' = j[1-n]$,

$$\tilde{c}^\dagger_{j,\uparrow}\,\tilde{c}^\dagger_{j,\downarrow}\,\tilde{n}_{j,\downarrow}\,\tilde{n}_{j,\uparrow} = \frac{1}{C_J}\,f^\dagger_{x_{j''},\,c2}\,f_{x_j,\,c0}\,f_{x_{j'},\,s1}\;f_{x_{j+1},\,c0}. \tag{52}$$

It should be mentioned that in spite of the annihilation of one $s1$ pseudofermion, this process does not involve the corresponding creation of a $s1$ pseudofermion hole. Indeed, it involves the annihilation of the site $j' = jn_\uparrow$ in the effective $s1$ lattice. Thus, when the initial ground state belongs to a $m = 0$ CPHS ensemble subspace, in spite of the annihilation of the $s1$ pseudofermion the excited state corresponds to a fully occupied $s1$ band, as the initial ground state.

A similar process gives rise to creation of a local $s2$ pseudofermion provided that creation of the two rotated-electron doubly-occupied sites is replaced by creation of two spin-down rotated electron singly occupied sites. However, in this case there is the possibility that one (or both) the spin-down spinons needed for creation of the local $s2$ pseudofermion is (or are) generated from annihilation of one (or two) ground-state $s1$ pseudofermion(s). Such processes can *dress* any rotated-electron process and are behind the occurrence of an infinite number of compatible J-CPHS ensemble subspaces for each local rotated-electron operator. These non-dominant pseudofermion processes do not obey the relation (45) (which is not an exact rotated-electron selection rule) and for all finite values of U/t amount to less than 6% of the rotated-electron spectral weight [22]. For instance, in order to create one spin-down rotated electron at the empty site j, in addition to the pseudofermion process (46) there is for instance a process corresponding to the creation of a $c0$ pseudofermion with the operator $f^\dagger_{x_j,\,c0}$ and of a $s2$ pseudofermion with the operator $f^\dagger_{x_{j''},\,s2}$ such that $j'' = j[n_\uparrow - n_\downarrow]$ and to the annihilation of a $s1$ pseudofermion with the operator $f^\dagger_{x_{j'},\,s1}$ such that $j' = jn_\uparrow$,

$$\tilde{c}^\dagger_{j,\downarrow}\,(1-\tilde{n}_{j,\uparrow}) = \frac{1}{C_J}\,f^\dagger_{x_{j''},\,s2}\,f_{x_{j'},\,s1}\,f^\dagger_{x_j,\,c0}. \tag{53}$$

We emphasize that the amount of spectral weight transferred from the ground state by the operator (46) is much larger than that transferred by the operator (53). Indeed, the J-CPHS ensemble subspace associated with the expression (46) belongs the dominant CPHS ensemble subspace of the local rotated-electron operator, whereas the J-CPHS ensemble subspace corresponding the expression (53) does not. Note that in the present case the two competing J-CPHS ensemble subspaces can have the same pseudofermion deviation numbers and values except for the occupancies of the $s1$ and $s2$ branches. Thus, the processes generated by the operators (46) and (53) correspond to J-CPHS ensemble subspaces belonging to different CPHS ensemble subspaces such that $\{\Delta N_{s1} = 1,\, N_{s2} = 0\}$ and $\{\Delta N_{s1} = -1,\, N_{s2} = 2\}$, respectively. Similar *dressing processes* involving creation of $s\nu$ pseudofermions belonging to $\nu > 1$ branches by annihilation of one to ν ground-state $s1$ pseudofermions can occur for all rotated-electron processes but correspond to very fast decreasing values of the amount of spectral weight transferred from the ground state for increasing number of pseudofermion processes [3,22]. Moreover, we recall that the subspace summation on the right-hand side of the spectral-function expression (36) is limited to the compatible CPHS ensemble subspaces: their pseudofermion number deviations and numbers obey the sum rules (18), (19), (39), and (43) and selection rules (21), (40), and (42).

We could present here other pseudofermion terms of increasing complexity, corresponding to the local rotated-electron operators considered above. However, the amount of spectral weight transferred from the ground state by the pseudofermion operator terms describing the above-mentioned dressing processes involving creation of $s\nu$ pseudofermions such that $\nu > 1$ by annihilation of an increasing number of ground-state $s1$ pseudofermions decreases very rapidly for increasing values of ν. Also the spectral weight transferred from the ground state by the operator terms with increasing value for the index i of the expression (32) of the general operator $\hat{\Theta}^l_{\mathcal{N},\,j}$ decreases very rapidly. For instance, for the one-electron spectral weight the contributions from dressing $s\nu$ pseudofermion processes for $\nu > 2$ and the terms of index $i > 1$ of the expression (32) for $\mathcal{N} = 1$ are typically beyond numerical measurability. Therefore, as far as numerical measurability is concerned, only a few pseudofermion terms contribute to the actual electronic spectral-weight distributions [3,22].

5 The spectral function as a convolution of pseudofermion spectral functions

In this section we express the spectral functions (37) as a convolution of pseudofermion, independent $-1/2$ holon, and independent $-1/2$ spinon spectral functions. The excited energy eigenstates appearing on the right-hand side of equation (37) can be written as the following pseudofermion Slater determinant,

$$|f.L,\, C\rangle = \prod_{\alpha\nu} F^{\dagger}_{f,\,\alpha\nu}|0\rangle;$$

$$F^{\dagger}_{f,\,\alpha\nu} = \prod_{\bar{q}_j=-q^0_{\alpha\nu}}^{+q^0_{\alpha\nu}} \Big[\mathcal{N}_{\alpha\nu}(\bar{q}_j)\, f^{\dagger}_{\bar{q},\,\alpha\nu} + [1-\mathcal{N}_{\alpha\nu}(\bar{q}_j)]\Big]. \tag{54}$$

Here and in other expressions below $|0\rangle$ is the pseudofermion vacuum such that $f_{\bar{q}_j,\,\alpha\nu}|0\rangle = 0$ for all $\alpha\nu$ branches and canonical-momentum values. In turn, according to equations (C.24) and (C.25) of reference [9], the ground state corresponds to a canonical-momentum densely packed occupancy for the $c0$ and $s1$ pseudofermion bands and the Slater determinant has the following simpler form,

$$|GS\rangle = \prod_{\alpha\nu=c0,\,s1} F^{\dagger}_{GS,\,\alpha\nu}|0\rangle;$$

$$F^{\dagger}_{GS,\,\alpha\nu} = \prod_{\bar{q}_j=-q^0_{F\alpha\nu}}^{+q^0_{F\alpha\nu}} f^{\dagger}_{\bar{q}_j,\,\alpha\nu}; \quad \alpha\nu = c0,\, s1;$$

$$F^{\dagger}_{0-GS,\,\alpha\nu} = \prod_{\bar{q}_j=q^0_{F\alpha\nu,\,-1}}^{q^0_{F\alpha\nu,\,+1}} f^{\dagger}_{\bar{q}_j,\,\alpha\nu}; \quad \alpha\nu = c0,\, s1;$$

$$F^{\dagger}_{J-GS,\,\alpha\nu} = \prod_{\bar{q}_j=\bar{q}_{F\alpha\nu,\,-1}}^{\bar{q}_{F\alpha\nu,\,+1}} f^{\dagger}_{\bar{q}_j,\,\alpha\nu}; \quad \alpha\nu = c0,\, s1. \tag{55}$$

The generators $F^{\dagger}_{0-GS,\,\alpha\nu}$ and $F^{\dagger}_{J-GS,\,\alpha\nu}$ given here correspond to densely packed distributions introduced below and the discrete canonical-momentum values of the pseudofermion operators $f^{\dagger}_{\bar{q}_j,\,\alpha\nu}$ of their expressions are those of the CPHS ensemble subspace which the ground state $|GS\rangle$ and the excited state $|f.L;\, C\rangle$ of equation (54) belong to, respectively. The *Fermi points* appearing in the products of their expressions of equation (55) read $q^0_{F\alpha\nu,\,\pm1} = \pm q^0_{F\alpha\nu} \pm [2\pi/L]\Delta N^{0,F}_{\alpha\nu,\,\pm1}$ and $\bar{q}_{F\alpha\nu,\,\pm1} = \pm q^0_{F\alpha\nu} \pm [2\pi/L][\Delta N^{F}_{\alpha\nu,\,\pm1} \pm Q^{\Phi}_{\alpha\nu}(\pm q^0_{F\alpha\nu})/2\pi]$, respectively, where the deviation numbers $\Delta N^{0,F}_{\alpha\nu,\pm1}$ and $\Delta N^{F}_{\alpha\nu,\pm1}$ are those of equation (35).

The excited-energy-eigenstate canonical-momentum distribution function $\mathcal{N}_{\alpha\nu}(\bar{q}_j)$ on the right-hand side of equation (54) can be written as,

$$\begin{aligned}
&\mathcal{N}_{\alpha\nu}(\bar{q}_j) = \mathcal{N}^{ph}_{\alpha\nu}(\bar{q}_j) + \Delta\mathcal{N}^{NF}_{\alpha\nu}(\bar{q}_j); \quad \alpha\nu = c0,\, s1;\\
&\mathcal{N}^{ph}_{\alpha\nu}(\bar{q}_j) = \mathcal{N}^{-0}_{\alpha\nu}(\bar{q}_j) + \Delta\mathcal{N}^{phF}_{\alpha\nu}(\bar{q}_j); \quad \alpha\nu = c0,\, s1;\\
&\mathcal{N}^{-0}_{\alpha\nu}(\bar{q}_j) = \mathcal{N}^{0}_{\alpha\nu}(\bar{q}_j) + \Delta\mathcal{N}^{F}_{\alpha\nu}(\bar{q}_j); \quad \alpha\nu = c0,\, s1;\\
&\mathcal{N}_{\alpha\nu}(\bar{q}_j) = \Delta\mathcal{N}^{NF}_{\alpha\nu}(\bar{q}_j) + \Delta\mathcal{N}^{F}_{\alpha\nu}(\bar{q}_j); \quad \alpha\nu \neq c0,\, s1.
\end{aligned} \tag{56}$$

Here $\mathcal{N}^{-0}_{\alpha\nu}(\bar{q}_j)$ and $N^{-0}_{\alpha\nu}(q_j)$, such that $\mathcal{N}^{-0}_{\alpha\nu}(\bar{q}_j) = N^{-0}_{\alpha\nu}(q_j)$, correspond to the excited densely packed distributions $\prod_{\alpha\nu=c0,\,s1} F^{\dagger}_{J-GS,\,\alpha\nu}|0\rangle$ and $\prod_{\alpha\nu=c0,\,s1} F^{\dagger}_{0-GS,\,\alpha\nu}|0\rangle$, respectively. Furthermore, the ground-state distribution $\mathcal{N}^{0}_{\alpha\nu}(\bar{q}_j)$ is both such that $\bar{q}_j = q_j$ and $\mathcal{N}^{0}_{\alpha\nu}(\bar{q}_j) = N^{0}_{\alpha\nu}(q_j)$, where $N^{0}_{\alpha\nu}(q_j)$ is the ground-state bare-momentum distribution function given in equations (C.1)–(C.3) of reference [9]. Thus, $\Delta\mathcal{N}^{F}_{\alpha\nu}(\bar{q}_j) = \Delta N^{F}_{\alpha\nu}(q_j)$ describes $\alpha\nu = c0,\, s1$ pseudofermion addition to or removal from the *Fermi points*. Moreover, $\Delta\mathcal{N}^{NF}_{\alpha\nu}(\bar{q}_j) = \Delta N^{NF}_{\alpha\nu}(\bar{q}_j)$ describes $\alpha\nu$ pseudofermion creation and/or annihilation away from the *Fermi points* for the $\alpha\nu = c0,\, s1$ branches and creation of $\alpha\nu$ pseudofermions at canonical-momentum values such that $|\bar{q}_j| < q^0_{\alpha\nu}$ for the $\alpha\nu \neq c0,\, s1$ branches, whereas for the latter branches $\Delta\mathcal{N}^{F}_{\alpha\nu}(\bar{q}_j) = \Delta N^{F}_{\alpha\nu}(\bar{q}_j)$ describes creation of $\alpha\nu \neq c0,\, s1$ pseudofermions at the limiting canonical-momentum values $\bar{q}_j = \pm q^0_{\alpha\nu}$. Finally, the deviation $\Delta\mathcal{N}^{phF}_{\alpha\nu}(\bar{q}_j) = \Delta N^{phF}_{\alpha\nu}(q_j)$ corresponds to low-energy and small-momentum $\alpha\nu = c0,\, s1$ pseudofermion particle-hole processes. For $n = 1$ (and/or $m = 0$) the excitation subspace is such that $\Delta\mathcal{N}^{phF}_{c0}(\bar{q}_j) = \Delta N^{phF}_{c0}(q_j) = 0$ (and/or $\Delta\mathcal{N}^{phF}_{s1}(\bar{q}_j) = \Delta N^{phF}_{s1}(q_j) = 0$). The above deviations are such that,

$$\sum_{\bar{q}_j=-q^0_{\alpha\nu}}^{+q^0_{\alpha\nu}} \Delta\mathcal{N}^{phF}_{\alpha\nu}(\bar{q}_j) = 0; \qquad \sum_{\bar{q}_j=-q^0_{\alpha\nu}}^{+q^0_{\alpha\nu}} \Delta\mathcal{N}^{NF}_{\alpha\nu}(\bar{q}_j) = \Delta N^{NF}_{\alpha\nu};$$

$$\sum_{\bar{q}_j=-q^0_{\alpha\nu}}^{+q^0_{\alpha\nu}} \Delta\mathcal{N}^{F}_{\alpha\nu}(\bar{q}_j) = \Delta N^{F}_{\alpha\nu}; \qquad \alpha\nu = c0,\, s1.$$

Since for the $\alpha\nu \neq c0,\, s1$ pseudofermion branches there is no occupancy in the initial ground state, the canonical-momentum distribution function is such that, $\sum_{\bar{q}_j=-q^0_{\alpha\nu}}^{+q^0_{\alpha\nu}} \Delta\mathcal{N}_{\alpha\nu}(\bar{q}_j) = N^{NF}_{\alpha\nu} + N^{F}_{\alpha\nu}$. [See Eq. (35).]

The generator $F^{\dagger}_{f,\,\alpha\nu}$ given in equation (54) can be written as,

$$\begin{aligned}
F^{\dagger}_{f,\,\alpha\nu} &= F^{\dagger}_{p-h,\,\alpha\nu}\, F^{\dagger}_{J-NF,\,\alpha\nu}\, F^{\dagger}_{J-GS,\,\alpha\nu}; \qquad \alpha\nu = c0,\, s1,\\
&= F^{\dagger}_{NF,\,\alpha\nu}\, F^{\dagger}_{F,\,\alpha\nu}; \qquad \alpha\nu \neq c0,\, s1.
\end{aligned}$$

The expressions of the generators $F^{\dagger}_{J-NF,\,\alpha\nu}$, $F^{\dagger}_{p-h,\,\alpha\nu}$, and $F^{\dagger}_{NF,\,\alpha\nu}$ in terms of pseudofermion creation and annihilation operators are given in equations (B.1), (B.4), and (B.5) of reference [3], respectively, and that of the generator $F^{\dagger}_{J-GS,\,\alpha\nu}$ is provided in equation (55), whereas

the generator $F^{\dagger}_{F,\alpha\nu}$ creates $\alpha\nu \neq c0, s1$ pseudofermions at $q = \pm q^0_{\alpha\nu}$. The generators $F^{\dagger}_{p-h,\alpha\nu}\, F^{\dagger}_{J-GS,\alpha\nu}$ and $F^{\dagger}_{J-NF,\alpha\nu}$ are associated with the deviations $\mathcal{N}^{ph}_{\alpha\nu}(\bar{q}_j)$ and $\Delta\mathcal{N}^{NF}_{\alpha\nu}(\bar{q}_j)$ of equation (56), respectively, $F^{\dagger}_{p-h,\alpha\nu}$ corresponds to the deviation $\Delta\mathcal{N}^{phF}_{\alpha\nu}(\bar{q}_j)$ of the same equation and thus generates the low-energy and small-momentum $\alpha\nu = c0, s1$ pseudofermion particle-hole processes (C). The operators $F^{\dagger}_{NF,\alpha\nu}$ and $F^{\dagger}_{F,\alpha\nu}$ refer to the $\alpha\nu \neq c0, s1$ branches and are associated with the deviations $\Delta\mathcal{N}^{NF}_{\alpha\nu}(\bar{q}_j)$ and $\Delta\mathcal{N}^{F}_{\alpha\nu}(\bar{q}_j)$, respectively.

The precise expression of the spectral functions of equation (37) depends on the specific form of the local operator $\tilde{\Theta}^{l}_{\mathcal{N}_i,j}$, whose expression includes contributions from all $\alpha\nu$ branches with finite pseudofermion occupancy in the corresponding J-CPHS ensemble subspace. For each such a subspace that operator expression has the following general form,

$$\tilde{\Theta}^{l}_{\mathcal{N}_i,j} = \frac{1}{G_C}\left[\prod_{\alpha\nu}\tilde{\Theta}^{l,i}_{j',\alpha\nu}\right], \qquad (57)$$

where the real positive number G_C whose expression is given below in equation (68) is that appearing in the general expression of the coefficient C_J provided in equation (46) and we recall that $j' = jn^*_{\alpha\nu}$ denotes the integer number closest to $jn^*_{\alpha\nu}$. In equation (57) and in the remaining of this paper $\theta(x)$ is such that $\theta(x) = 1$ for $x > 0$ and $\theta(x) = 0$ for $x \leq 0$.

As mentioned in Section 4, the value of the coefficient G_C appearing in the general expression for the operator $\tilde{\Theta}^{l}_{\mathcal{N}_i,j}$ given in equation (57) is the same for all J-CPHS ensemble subspaces belonging to a given CPHS ensemble subspace, whereas that of the real positive numbers G_J and $|C_J|$ of equation (46) is specific to each J-CPHS ensemble subspace. Furthermore, when the expression of the local operator $\hat{O}^{l}_{\mathcal{N},j}$ of equation (7) is independent of U/t, the same occurs for the related operators $\hat{\Theta}^{l}_{\mathcal{N},j}$ and $\tilde{\Theta}^{l}_{\mathcal{N}_0,j}$ of equations (27, 28) and (32), respectively. It follows that in the case of the $i = 0$ operator $\tilde{\Theta}^{l}_{\mathcal{N}_0,j}$, the value of the coefficient G_C appearing in its expression given in equation (57) is also independent of U/t. Fortunately, for the dominant CPHS ensemble subspaces considered in the previous section, such a value can be found from analysis of the problem for $U/t = 0$ or $U/t = \infty$. One then finds that $G_C = 1$ in the $\tilde{\Theta}^{l}_{\mathcal{N}_0,j} = \frac{1}{G_C}[\prod_{\alpha\nu}\tilde{\Theta}^{l,0}_{j',\alpha\nu}]$ expression corresponding to the dominant CPHS ensemble subspaces, as pointed out in Section 4.

The operator $\tilde{\Theta}^{l,i}_{j',\alpha\nu}$ appearing in equation (57) has the following general form for the $\alpha\nu$ branches with finite pseudofermion occupancy in the J-CPHS subspace,

$$\tilde{\Theta}^{l,i}_{j',\alpha\nu} = e^{-i\Delta P^0_{\alpha\nu}j'a^0_{\alpha\nu}}\,\tilde{\Theta}^{l,NF,i}_{j',\alpha\nu}\,\tilde{\Theta}^{l,F,i}_{\alpha\nu}.$$

Here the operators $\tilde{\Theta}^{l,NF,i}_{j',\alpha\nu}$ and $\tilde{\Theta}^{l,F,i}_{\alpha\nu}$ are associated with the elementary processes (A) and (B), respectively, and the *phase-factor momentum* $l\Delta P^0_{\alpha\nu}$ is given below. Considering that $[x_{j'} - x_j] = 0$, it is such that $-i\sum_{\alpha\nu}\Delta P^0_{\alpha\nu}j'a^0_{\alpha\nu} = -ij\Delta P_J$. Here the summation $\sum_{\alpha\nu}$ is over the $\alpha\nu$ branches with pseudofermion occupancy in the J-CPHS ensemble subspace and ΔP_J is the momentum deviation of the coefficient $C_J = e^{i\,j\Delta P_J}\,[G_C/G_J]$ given in equation (46), which reads,

$$\Delta P_J = \sum_{\alpha\nu}\Delta P^0_{\alpha\nu}.$$

Let us proceed by studying the phase factor $e^{-i\Delta P^0_{\alpha\nu}j'a^0_{\alpha\nu}}$ and operators $\tilde{\Theta}^{l,F,i}_{\alpha\nu}$ and $\tilde{\Theta}^{l,NF,i}_{j',\alpha\nu}$ whose product gives the operator $\tilde{\Theta}^{l,i}_{j',\alpha\nu}$. We start by characterizing for each $\alpha\nu$ branch the elementary processes that originate the phase factor $e^{-i\Delta P^0_{\alpha\nu}j'a^0_{\alpha\nu}}$. The expression of the local operator $\tilde{\Theta}^{l,i}_{j',\alpha\nu}$ does not involve the generator of the elementary processes (C), $F^{\dagger}_{p-h,\alpha\nu}$, but provides the momentum $l\Delta P^{phF}_{\alpha\nu}$ for such processes through a phase factor, $e^{-i\Delta P^{phF}_{\alpha\nu}j'a^0_{\alpha\nu}}$. Here $l\Delta P^{phF}_{\alpha\nu} = l[2\pi/L]\,[m_{\alpha\nu,+1} - m_{\alpha\nu,-1}]$ is the small momentum deviation generated by the $\alpha\nu = c0, s1$ pseudofermion particle-hole elementary processes (C) and $m_{\alpha\nu,\pm1}$ is the number of such processes of momentum $\pm[2\pi/L]$ in the vicinity of the Fermi points $\pm q^0_{F\alpha\nu}$. Furthermore, each $\alpha\nu = c0, s1$ pseudofermion created or annihilated at the *Fermi point* $\iota\, q^0_{F\alpha\nu}$ by the elementary processes (B) contributes with a phase factor $e^{-i\iota\, q^0_{F\alpha\nu}j'a^0_{\alpha\nu}}$ or $e^{+i\iota\, q^0_{F\alpha\nu}j'a^0_{\alpha\nu}}$, respectively, where $\iota = \pm1$. This leads to a phase factor $e^{-i2q^0_{F\alpha\nu}\Delta J^{0,F}_{\alpha\nu}j'a^0_{\alpha\nu}}$, where $2\Delta J^{0,F}_{\alpha\nu} = \Delta N^{0,F}_{\alpha\nu,+1} - \Delta N^{0,F}_{\alpha\nu,-1}$ and the number deviation $\Delta N^{0,F}_{\alpha\nu,\pm1}$ is that defined in equation (35). Moreover, each $c\nu \neq c0$ and $s\nu \neq s1$ FP current scattering center created by the elementary processes (B) contributes with a phase factor $e^{-i\iota\, q^0_{Fc0}j'a^0_{c0}}$ and $e^{-i\iota\, q^0_{Fc0}j'a^0_{c0}}\, e^{+i\iota\, 2q^0_{Fs1}j'a^0_{s1}}$, respectively. On the other hand, the scatter-less bare-momentum shift contributes with a phase factor $e^{-i[Q^0_{\alpha\nu}/L]j'a^0_{c\nu}}$ for each of the $N^0_{\alpha\nu}$ pseudofermions of the initial ground state, what gives $[e^{-i[Q^0_{\alpha\nu}/L]j'a^0_{c\nu}}]^{N^0_{\alpha\nu}} = e^{-iq^0_{F\alpha\nu}[Q^0_{\alpha\nu}/\pi]j'a^0_{c\nu}}$ with $\alpha\nu = c0, s1$. Adding all these contributions leads to the above net phase factor $e^{-i\Delta P^0_{\alpha\nu}j'a^0_{\alpha\nu}}$ for the $\alpha\nu = c0, s1$ branches whose phase-factor momentum reads $l\Delta P^0_{\alpha\nu} = l[\Delta P^{phF}_{\alpha\nu} + \Delta P^{F}_{\alpha\nu}]$. For densities in the ranges $0 < n < 1$ and $0 < m < n$, the momentum $\Delta P^F_{\alpha\nu}$ appearing in that phase factor is given by $\Delta P^F_{c0} = 4k_F[\,\Delta J^F_{c0} + \sum_{\nu=1}^{\infty} J^F_{c\nu} + \sum_{\nu=2}^{\infty} J^F_{s\nu}]$ and $\Delta P^F_{s1} = 2k_{F\downarrow}[\,\Delta J^F_{s1} - 2\sum_{\nu=2}^{\infty} J^F_{s\nu}]$ for the $\alpha\nu = c0$ and $\alpha\nu = s1$ branches, respectively. It results from the current contributions associated with the $c0$ and $s1$ *Fermi points* $\pm2k_F$ and $\pm k_{F\downarrow}$, respectively. Moreover, each $c\nu \neq c0$ pseudofermion created by the elementary processes (A) contributes with a phase factor $e^{-i(1+\nu)\pi j'a^0_{c\nu}}$ what leads to a net phase factor $e^{-i\Delta P^0_{c\nu}j'a^0_{c\nu}}$ for the $c\nu \neq c0$ branches such that $\Delta P^0_{c\nu} = (1+\nu)\pi\mathcal{N}_{c\nu}$. Finally, the phase-factor momentum vanishes for the $s\nu \neq s1$ branches. Thus, the phase-factor momenta contributing to ΔP_J read,

$$l\Delta P^0_{\alpha\nu} = l[\Delta P^{phF}_{\alpha\nu} + \Delta P^{F}_{\alpha\nu}], \quad \alpha\nu = c0, s1;$$
$$l\Delta P^0_{c\nu} = l(1+\nu)\pi\mathcal{N}_{c\nu}, \quad c\nu \neq c0; \quad l\Delta P^0_{s\nu} = 0, \ s\nu \neq s1.$$

Next we consider the operator $\tilde{\Theta}^{l,F,i}_{\alpha\nu}$. For the $c\nu \neq c0$ and $s\nu \neq s1$ branches, that operator creates $2\nu N^F_{c\nu}$ independent $-1/2$ holons of momentum π and $2\nu N^F_{s\nu}$ independent $-1/2$ spinons of momentum zero, respectively. (The only effect of the creation of the corresponding $N^F_{c\nu}$ $c\nu \neq c0$ FP current scattering centers and $N^F_{s\nu}$ $s\nu \neq s1$ FP current scattering centers [10], respectively, is the above contribution to the phase factor $e^{-i\Delta P^0_{c0} j' a^0_{c0}}$ and $e^{-i\Delta P^0_{c0} j' a^0_{c0}} e^{-i\Delta P^0_{s1} j' a^0_{s1}}$, respectively.) For the $\alpha\nu = c0,\ s1$ branches the operator $\tilde{\Theta}^{l,F,i}_{\alpha\nu}$ is such that,

$$e^{-i2q^0_{\alpha\nu}\Delta J^{0,F}_{\alpha\nu} j' a^0_{\alpha\nu}}\,\tilde{\Theta}^{l,F,i}_{\alpha\nu} = \left(\frac{1}{N^*_{\alpha\nu}}\right)^{\frac{|\Delta N^F_{\alpha\nu}|}{2}} \times \prod_{\iota=\pm 1}\left\{\Theta(\Delta N^F_{\alpha\nu,\,\iota}) \prod_{i'=1}^{\Delta N^F_{\alpha\nu,\,\iota}}\left[\sum_{j''=1}^{N^*_{\alpha\nu}} e^{-i\iota(q^0_{\alpha\nu}+2\pi\, i'/L)a^0_{\alpha\nu}(j'-j'')} \times f^\dagger_{x_{j''},\,\alpha\nu}\right] + \Theta(-\Delta N^F_{\alpha\nu,\,\iota}) \times \prod_{i'=0}^{|\Delta N^F_{\alpha\nu,\,\iota}|-1}\left[\sum_{j''=1}^{N^*_{\alpha\nu}} e^{i\iota(q^0_{\alpha\nu}-2\pi\, i'/L)a^0_{\alpha\nu}(j'-j'')} f_{x_{j''},\,\alpha\nu}\right]\right\};\quad \alpha\nu = c0,\ s1.$$

Thus, that operator can be written as,

$$\tilde{\Theta}^{l,F,i}_{\alpha\nu} = \prod_{\iota=\pm 1}\Big\{\,\Theta(\Delta N^F_{\alpha\nu,\,\iota}) \prod_{i'=1}^{\Delta N^F_{\alpha\nu,\,\iota}} f^\dagger_{\iota(q^0_{\alpha\nu}+2\pi\, i'/L),\,\alpha\nu} + \Theta(-\Delta N^F_{\alpha\nu,\,\iota}) \prod_{i'=0}^{|\Delta N^F_{\alpha\nu,\,\iota}|-1} f_{\iota(q^0_{\alpha\nu}-2\pi\, i'/L),\,\alpha\nu}\Big\};\ \alpha\nu = c0,\ s1,$$

where we omitted corrections of order $1/L$ to the momentum value $q^0_{\alpha\nu}$ appearing in the phase factor. However, these corrections must be considered in the momentum of the pseudofermion operators. In the above two equations the pseudofermion operators correspond to spatial and canonical-momentum variables, respectively, and in the argument of the exponentials appearing in these equations and in other equations given below i is the usual imaginary number. (It is not the index i of the operator $\tilde{\Theta}^{l,F,i}_{\alpha\nu}$, whereas i' is a summation index.) Moreover, in the above equations and in the remaining of this paper $\Theta(x)$ is such that $\Theta(x) = 1$ for $x \geq 0$ and $\Theta(x) = 0$ for $x < 0$.

We finish the study of the operator $\tilde{\Theta}^{l,i}_{j',\,\alpha\nu}$ by considering the operator $\tilde{\Theta}^{l,NF,i}_{j',\,\alpha\nu}$ associated with the elementary processes (A), whose expression refers to a given J-CPHS subspace. In order to arrive to that expression in terms of the local $\alpha\nu$ pseudofermion creation and annihilation operators, we recall that our study refers to spectral functions of form (7) whose operator $\hat{O}^l_{\mathcal{N},\,j}$ expression involves $\mathcal{N}$ elementary electronic operators which create or annihilate electrons in a compact domain of lattice sites. For such an operator the general expression of the corresponding operators $\tilde{\Theta}^{l,NF,i}_{j',\,\alpha\nu}$ involves $\mathcal{N}_{\alpha\nu}$ local $\alpha\nu$ pseudofermion creation and annihilation operators for the $\alpha\nu = c0,\ s1$ branches (and creation operators for the $\alpha\nu \neq c0,\ s1$ branches) which refer to a compact domain of $\mathcal{N}_{\alpha\nu}$ effective $\alpha\nu$ lattice sites. The operators (46)–(53) involve the product of operators whose expressions involve elementary operators of a single $\alpha\nu$ branch and except for a multiplicative constant are particular examples of such a general expression, which has the following form,

$$\tilde{\Theta}^{l,NF,i}_{j',\,\alpha\nu} = (n^*_{\alpha\nu})^{\frac{\mathcal{N}_{\alpha\nu}-1}{2}}\Bigg[\Theta(\Delta N^{NF}_{\alpha\nu}) \times \prod_{j''=j'}^{\Delta N^{NF}_{\alpha\nu}+N^{phNF}_{\alpha\nu}+j'-1}\ \prod_{j'''=\Delta N^{NF}_{\alpha\nu}+N^{phNF}_{\alpha\nu}+j'}^{\mathcal{N}_{\alpha\nu}+j'-1} f^\dagger_{x_{j''},\,\alpha\nu}\, f_{x_{j'''},\,\alpha\nu} + \theta(-\Delta N^{NF}_{\alpha\nu}) \times \prod_{j''=j'}^{|\Delta N^{NF}_{\alpha\nu}|+N^{phNF}_{\alpha\nu}+j'-1}\ \prod_{j'''=|\Delta N^{NF}_{\alpha\nu}|+N^{phNF}_{\alpha\nu}+j'}^{\mathcal{N}_{\alpha\nu}+j'-1} f_{x_{j''},\,\alpha\nu}\, f^\dagger_{x_{j'''},\,\alpha\nu}\Bigg];$$

$\alpha\nu = c0,\ s1,$

and

$$\tilde{\Theta}^{l,NF,i}_{j',\,\alpha\nu} = (n^*_{\alpha\nu})^{\frac{\mathcal{N}_{\alpha\nu}-1}{2}} \prod_{j''=j'}^{\mathcal{N}_{\alpha\nu}+j'-1} f^\dagger_{x_{j''},\,\alpha\nu};\quad c\nu \neq c0,\ n < 1;\quad s\nu \neq s1,\ m < n.$$

Here the spatial coordinates $x_0,\ x_1,...,x_{\mathcal{N}_{\alpha\nu}-1}$ correspond to the compact domain of $\mathcal{N}_{\alpha\nu}$ effective $\alpha\nu$ lattice sites where the number $\mathcal{N}_{\alpha\nu}$ is given in equation (46).

Let us consider the operator $\tilde{\Theta}^{l,i}_{k,\,\alpha\nu}$, which is the Fourier transform of the above local operator $\tilde{\Theta}^{l,i}_{j',\,\alpha\nu}$,

$$\tilde{\Theta}^{l,i}_{k,\,\alpha\nu} = \frac{1}{\sqrt{N^*_{\alpha\nu}}} \sum_{j'=1}^{N^*_{\alpha\nu}} e^{+i\,lkj' a^0_{\alpha\nu}}\,\tilde{\Theta}^{l,i}_{j',\,\alpha\nu}.$$

This operator can be expressed in terms of the following momentum convolution,

$$\tilde{\Theta}^{l,i}_{k,\,\alpha\nu} = \sum_{k'} \tilde{\Theta}^{l,NF,i}_{k-k',\,\alpha\nu}\,\tilde{\Theta}^{l,F,i}_{\alpha\nu}\,\delta_{k',\,l\Delta P^0_{\alpha\nu}} = \tilde{\Theta}^{l,NF,i}_{k-l\Delta P^0_{\alpha\nu},\,\alpha\nu}\tilde{\Theta}^{l,F,i}_{\alpha\nu},$$

where the operator $\tilde{\Theta}^{l,F,i}_{\alpha\nu}$ was given above and $\tilde{\Theta}^{l,NF,i}_{k,\,\alpha\nu}$ is the Fourier transform of the local operator $\tilde{\Theta}^{l,NF,i}_{j',\,\alpha\nu}$. It

reads,

$$\tilde{\Theta}^{l,NF,i}_{k,\,\alpha\nu} = \left(\frac{1}{N_a}\right)^{\frac{\mathcal{N}_{\alpha\nu}-1}{2}} \left\{ \Theta(\Delta N^{NF}_{\alpha\nu}) \left[\prod_{i'=0}^{\Delta N^{NF}_{\alpha\nu}+N^{phNF}_{\alpha\nu}-1} \right.\right.$$
$$\times \prod_{i''=\Delta N^{NF}_{\alpha\nu}+N^{phNF}_{\alpha\nu}}^{\mathcal{N}_{\alpha\nu}-1} \left(\sum_{\bar{q}_{i'}=-q^0_{\alpha\nu}}^{+q^0_{\alpha\nu}} e^{-ii'a^0_{\alpha\nu}\bar{q}_{i'}}\, f^\dagger_{\bar{q}_{i'},\,\alpha\nu} \right)$$
$$\left.\left. \times \left(\sum_{\bar{q}_{i''}=-q^0_{\alpha\nu}}^{+q^0_{\alpha\nu}} e^{ii''a^0_{\alpha\nu}\bar{q}_{i''}}\, f_{\bar{q}_{i''},\,\alpha\nu} \right) \right]$$
$$\times \delta_{k,\,l[\sum_{i'=0}^{\Delta N^{NF}_{\alpha\nu}+N^{phNF}_{\alpha\nu}-1}\bar{q}_{i'}-\sum_{i''=\Delta N^{NF}_{\alpha\nu}+N^{phNF}_{\alpha\nu}}^{\mathcal{N}_{\alpha\nu}-1}\bar{q}_{i''}]}$$
$$+\,\theta(-\Delta N^{NF}_{\alpha\nu}) \left[\prod_{i'=0}^{|\Delta N^{NF}_{\alpha\nu}|+N^{phNF}_{\alpha\nu}-1} \right.$$
$$\times \prod_{i''=|\Delta N^{NF}_{\alpha\nu}|+N^{phNF}_{\alpha\nu}}^{\mathcal{N}_{\alpha\nu}-1} \left(\sum_{\bar{q}_{i'}=-q^0_{\alpha\nu}}^{+q^0_{\alpha\nu}} e^{ii'a^0_{\alpha\nu}\bar{q}_{i'}}\, f_{\bar{q}_{i'},\,\alpha\nu} \right)$$
$$\left. \left. \times \left(\sum_{\bar{q}_{i''}=-q^0_{\alpha\nu}}^{+q^0_{\alpha\nu}} e^{-ii''a^0_{\alpha\nu}\bar{q}_{i''}}\, f^\dagger_{\bar{q}_{i''},\,\alpha\nu} \right) \right] \right\}$$
$$\times \delta_{k,\,l[-\sum_{i'=0}^{|\Delta N^{NF}_{\alpha\nu}|+N^{phNF}_{\alpha\nu}-1}\bar{q}_{i'}+\sum_{i''=|\Delta N^{NF}_{\alpha\nu}|+N^{phNF}_{\alpha\nu}}^{\mathcal{N}_{\alpha\nu}-1}\bar{q}_{i''}]};$$
$$\alpha\nu = c0,\, s1$$

$$\tilde{\Theta}^{l,NF,i}_{k,\,\alpha\nu} = \left(\frac{1}{N_a}\right)^{\frac{\mathcal{N}_{\alpha\nu}-1}{2}} \left[\prod_{i'=0}^{\mathcal{N}_{\alpha\nu}-1} \sum_{\bar{q}_{i'}=-q^0_{\alpha\nu}}^{+q^0_{\alpha\nu}} e^{-ii'a^0_{\alpha\nu}\bar{q}_{i'}}\, f^\dagger_{\bar{q}_{i'},\,\alpha\nu} \right]$$
$$\times \delta_{k,\,l[c_{\alpha\nu}\sum_{i'=0}^{\mathcal{N}_{\alpha\nu}-1}\bar{q}_{i'}]}; \qquad c\nu \neq c0, \quad n < 1;$$
$$s\nu \neq s1, \quad m > 0. \quad (58)$$

Here the set $\bar{q}_0,\ \bar{q}_1,\ \bar{q}_2$,...,$\bar{q}_{\mathcal{N}_{\alpha\nu}-1}$ refers to $\mathcal{N}_{\alpha\nu}$ summation canonical-momentum variables associated with the $\alpha\nu$ pseudofermion bands. We note that the canonical-momentum values in the Krönecker δ's of equation (58) run under the summations but not under the products appearing in that equation. For the $\alpha\nu \neq c0,\, s1$ branches, the $\mathcal{N}_{\alpha\nu}$-$\alpha\nu$ pseudofermion operator $\tilde{\Theta}^{l,NF,i}_{k,\,\alpha\nu}$ creates and annihilates $|\Delta N^{NF}_{\alpha\nu}|$ $\alpha\nu$ pseudofermions when $\Delta N^{NF}_{\alpha\nu} > 0$ and $\Delta N^{NF}_{\alpha\nu} < 0$, respectively, and generates $N^{phNF}_{\alpha\nu} = 0, 1, ...$ finite-momentum and finite-energy $\alpha\nu$ pseudofermion particle-hole processes. For the $\alpha\nu \neq c0,\, s1$ branches, it creates $N^{NF}_{\alpha\nu}$ $\alpha\nu$ pseudofermions of bare-momentum q such that $|q| < q^0_{\alpha\nu}$.

In the case of the $\alpha\nu \neq c0,\, s1$ branches, the general expression given in equation (58) for the operator $\tilde{\Theta}^{l,NF,i}_{k,\,\alpha\nu}$ is valid for densities such that the corresponding ratios $n^*_{\alpha\nu} = N^*_{\alpha\nu}/N_a$ have finite values. For the $c\nu \neq c0$ (and $s\nu \neq s1$) pseudofermion branches and electronic density $n = 1$ (and spin density $m = 0$) all pseudofermions separate into 2ν independent $-1/2$ holons (and 2ν independent $-1/2$ spinons). Therefore, the operator given in equation (58) does not exist. Moreover, for $n = 1$ (and $m = 0$) the above generator $F^\dagger_{p-h,\,c0}$ (and $F^\dagger_{p-h,\,s1}$) of the elementary processes (C) reduces to $F^\dagger_{p-h,\,c0} = 1$ (and $F^\dagger_{p-h,\,s1} = 1$). However, our theory also applies for electronic density $n = 1$ (and spin density $m = 0$), provided that we consider the corresponding restrictions in the $c0$ (and $s1$) excitation spectrum and take into account that $\tilde{\Theta}^{l,i}_{k,\,\alpha\nu} = \tilde{\Theta}^{l,NF,i}_{k,\,\alpha\nu}$, for the $c\nu \neq c0$ (and $s\nu \neq s1$) branches.

For the $\alpha\nu = c0,\, s1$ branches the pseudofermion weight distribution involves the following matrix element,

$$\langle 0|F_{J-GS,\,\alpha\nu}\, F_{J-NF,\,\alpha\nu}\, F_{p-h,\,\alpha\nu}\, \tilde{\Theta}^{l,i}_{k,\,\alpha\nu}\, F^\dagger_{GS,\,\alpha\nu}|0\rangle; \qquad \alpha\nu = c0,\, s1.$$

Our study refers to very large values of L when the commutator $[F^\dagger_{p-h,\,\alpha\nu},\, F^\dagger_{J-NF,\,\alpha\nu}] = 0$ vanishes and the operator $\tilde{\Theta}^{l,F,i}_{\alpha\nu}$ is such that $\tilde{\Theta}^{l,F,i}_{\alpha\nu}\, F^\dagger_{GS,\,\alpha\nu} = F^\dagger_{0-GS,\,\alpha\nu}$ and thus the matrix element can be rewritten as,

$$\langle 0|F_{J-GS,\,\alpha\nu}\, F_{p-h,\,\alpha\nu}\, F_{J-NF,\,\alpha\nu}\tilde{\Theta}^{l,NF,i}_{k-l\Delta P^0_{\alpha\nu},\,\alpha\nu}\, F^\dagger_{0-GS,\,\alpha\nu}|0\rangle; \qquad \alpha\nu = c0,\, s1.$$

When applying the generators $F^\dagger_{f,\,L,\,\alpha\nu}$ and $F^\dagger_{GS,\,\alpha\nu}$ of equations (54) and (55), respectively, onto the pseudofermion vacuum to construct a given energy eigenstate, the set of $\alpha\nu$ band discrete canonical-momentum values $\{\bar{q}_j\}$ of the pseudofermion operators $f^\dagger_{\bar{q}_j,\,\alpha\nu}$ in the expressions of these generators are those of the CPHS ensemble subspace which that state belongs to. This rule applies when one considers the generators of the full energy eigenstates. (Below we express each J-CPHS as a direct product of subspaces. To reach the correct final results, such a rule does not apply to some of the states which span such direct-product subspaces.) The same occurs with the discrete canonical-momentum values of the pseudofermion creation and annihilation operators of the expression of any operator $\tilde{\Theta}$ when it acts onto a given energy eigenstate. For instance, let $|\beta\rangle$ and $|\beta'\rangle$ be energy eigenstates. Thus, the discrete canonical-momentum values of the pseudofermion creation and annihilation operators of the expression of the operators $\tilde{\Theta}^\dagger$ and $\tilde{\Theta}$ in $\tilde{\Theta}^\dagger|\beta'\rangle$ and $\tilde{\Theta}|\beta\rangle$ are those of the CPHS ensemble subspace which the states $|\beta'\rangle$ and $|\beta\rangle$ belong to, respectively. An important property for our theory is that for L large both choices lead to the same value for the matrix element $\langle\beta|\tilde{\Theta}|\beta'\rangle$.

The operator $\tilde{\Theta}^{l,NF,i}_{k,\,\alpha\nu}$ of equation (58) is for the $\alpha\nu = c0,\, s1$ branches such that the commutator $[F_{p-h,\,\alpha\nu},\, \tilde{\Theta}^{l,NF,i}_{k,\,\alpha\nu}] = 0$ vanishes when it acts onto the CPHS ensemble subspace which the corresponding excited state belongs to. Furthermore, there occurs a full overlap of that operator with the generator $F_{J-NF,\,\alpha\nu}$ and for the $\alpha\nu \neq c0,\, s1$ branches there occurs a full overlap of the operator $\tilde{\Theta}^{l,NF,i}_{k,\,\alpha\nu}$ given in the second expression of equation (58) with the generator $F_{NF,\,\alpha\nu}$. The latter full overlap results from the lack of $\alpha\nu \neq c0,\, s1$ pseudofermion occupancy of the initial ground state.

A J-CPHS ensemble subspace can be expressed as the direct product of subspaces, one for each $\alpha\nu$ branch

pseudofermion occupancy. In the particular case of the $\alpha\nu = c0,\, s1$ branches the low-energy and high-energy physics separate provided that L is large and one can define two of such product subspaces for each branch. They are associated with the excitation occupancy configurations generated by the finite-energy elementary processes (A) and low-energy elementary processes (B, C), respectively. We call $p-h, \alpha\nu = c0,\, s1$ branch subspace the latter low-energy subspace. Thus, the number of product subspaces equals the number of $\alpha\nu$ branches with finite pseudofermion occupancy in the J-CPHS ensemble subspace plus two. Finally, for some J-CPHS ensemble subspaces the direct product also includes the independent $-1/2$ holon subspace and independent $-1/2$ spinon subspace. For such subspaces the generator $F^{\dagger}_{F,\,\alpha\nu}$ either creates $N^{F}_{\alpha\nu}$ $\alpha\nu$ pseudofermions with limiting bare-momentum values $q = \pm q^{0}_{\alpha\nu}$ or reads $F^{\dagger}_{F,\,\alpha\nu} = 1$ when $N^{F}_{\alpha\nu} = 0$ and thus $F^{\dagger}_{f,\,\alpha\nu} = F^{\dagger}_{NF,\,\alpha\nu}$ (or $F^{\dagger}_{f,\,\alpha\nu}$ does not exist if $n = 1$ and $\alpha\nu = c\nu$ or $m = 0$ and $\alpha\nu = s\nu$). The states which span the $\alpha\nu$ branch direct-product subspaces and $p-h, \alpha\nu = c0,\, s1$ branch direct-product subspaces have the following form,

$$|f.L;\, \alpha\nu\rangle \equiv F^{\dagger}_{J-NF,\,\alpha\nu}|GS\rangle; \quad \alpha\nu = c0,\, s1;$$

$$|f.L;\, \alpha\nu\rangle \equiv F^{\dagger}_{NF,\,\alpha\nu}|GS\rangle; \quad \alpha\nu \neq c0,\, s1;$$

$$|f.L;\, p-h, \alpha\nu\rangle \equiv F^{\dagger}_{p-h,\,\alpha\nu}\, F^{\dagger}_{J-GS,\,\alpha\nu}|0\rangle; \quad \alpha\nu = c0,\, s1.$$

Below we express the spectral functions as convolutions of $p-h$, $\alpha\nu$ and $\alpha\nu$ pseudofermion spectral functions. However, in order to reach the same spectral-weight distributions as by use of the above matrix elements, it turns out that:

(i) when applying the generators $F^{\dagger}_{J-NF,\,\alpha\nu}$ and $F^{\dagger}_{NF,\,\alpha\nu}$ onto the ground state $|GS\rangle$ to construct a given $\alpha\nu$ branch direct-product-subspace state, the set of the $\alpha\nu$ band discrete canonical-momentum values $\{\bar{q}_j\}$ of the pseudofermion operators $f^{\dagger}_{\bar{q}_j,\,\alpha\nu}$ in the expressions of these generators must be those of the ground-state CPHS ensemble subspace;

(ii) when applying the generator $F^{\dagger}_{p-h,\,\alpha\nu}\, F^{\dagger}_{J-GS,\,\alpha\nu}$ onto the pseudofermion vacuum $|0\rangle$ to construct a given $p-h, \alpha\nu = c0,\, s1$ branch direct-product-subspace state, the set of the $\alpha\nu$ band discrete canonical-momentum values $\{\bar{q}_j\}$ of the pseudofermion operators $f^{\dagger}_{\bar{q}_j,\,\alpha\nu}$ in the expressions of that generator must be those of the corresponding excited energy eigenstate.

The property (i) ensures that the above full matrix-element overlaps are reproduced. Furthermore, properties (i) and (ii) also ensure that the contribution from the unconventional orthogonality catastrophe matrix-element overlap discussed below is not counted twice.

Below we introduce the $\alpha\nu = c0,\, s1$ pseudofermion spectral functions and $p-h, \alpha\nu = c0,\, s1$ pseudofermion spectral functions which involve the operators $\tilde{\Theta}^{l,NF,i}_{k-l\Delta P^{F}_{\alpha\nu},\,\alpha\nu}$ and $\tilde{\Theta}^{l,F,i}_{\alpha\nu}\,\delta_{k',\,l\Delta P^{phF}_{\alpha\nu}}$, respectively. The momentum convolution of these two operators leads to the correct expression for the operator $\tilde{\Theta}^{l,i}_{k,\,\alpha\nu}$ such that $\tilde{\Theta}^{l,i}_{k,\,\alpha\nu} = \sum_{k'}\tilde{\Theta}^{l,NF,i}_{k-l\Delta P^{F}_{\alpha\nu}-k',\,\alpha\nu}\,\tilde{\Theta}^{l,F,i}_{\alpha\nu}\,\delta_{k',\,l\Delta P^{phF}_{\alpha\nu}} = \tilde{\Theta}^{l,NF,i}_{k-l\Delta P^{0}_{\alpha\nu},\,\alpha\nu}\,\tilde{\Theta}^{l,F,i}_{\alpha\nu}$. In turn, the $\alpha\nu \neq c0,\, s1$ pseudofermion spectral functions considered below correspond to the operators $\tilde{\Theta}^{l,NF,i}_{k-l\Delta P^{0}_{\alpha\nu},\,\alpha\nu}$, which refer to the $\alpha\nu \neq c0,\, s1$ branch direct-product subspaces. For the latter branches, the pseudofermion spectral function is associated with the $\mathcal{N}_{\alpha\nu} = N^{NF}_{\alpha\nu} > 0$ $\alpha\nu$ pseudofermions created by the processes (A), whereas the $N^{F}_{\alpha\nu}$ $\alpha\nu$ pseudofermions of limiting canonical momentum $\pm q^{0}_{\alpha\nu}$ contribute to the independent $-1/2$ holon ($\alpha\nu = c\nu$) or $-1/2$ spinon ($\alpha\nu = s\nu$) spectral function and to the momentum of the $\alpha\nu = c0,\, s1$ spectral functions associated with the elementary processes (A), through the FP-current-scattering-center phase factors.

The operators associated with the pseudofermion spectral functions can be written in the corresponding direct-product subspaces as,

$$\tilde{\Theta}^{l,NF,i}_{k-l\Delta P^{F}_{\alpha\nu},\,\alpha\nu} = \sum_{f}\langle f.L;\, \alpha\nu|\tilde{\Theta}^{l,NF,i}_{k-l\Delta P^{F}_{\alpha\nu},\,\alpha\nu}|GS\rangle\,|f.L;\, \alpha\nu\rangle\langle GS|; \quad \alpha\nu = c0,\, s1,$$

$$\tilde{\Theta}^{l,NF,i}_{k-l\Delta P^{0}_{\alpha\nu},\,\alpha\nu} = \sum_{f}\langle f.L;\, \alpha\nu|\tilde{\Theta}^{l,NF,i}_{k-l\Delta P^{0}_{\alpha\nu},\,\alpha\nu}|GS\rangle\,|f.L;\, \alpha\nu\rangle\langle GS|; \quad \alpha\nu \neq c0,\, s1,$$

$$\tilde{\Theta}^{l,F,i}_{\alpha\nu}\,\delta_{k,\,l\Delta P^{phF}_{\alpha\nu}} = \sum_{f}\langle f.L;\, p-h, \alpha\nu|\tilde{\Theta}^{l,F,i}_{\alpha\nu}|GS\rangle\delta_{k,\,l\Delta P^{phF}_{\alpha\nu}}\,|f.L;\, p-h, \alpha\nu\rangle\langle GS|; \quad \alpha\nu = c0,\, s1.$$

Here the f summations run over the states which span such subspaces and the matrix elements are given by,

$$\langle f.L;\, \alpha\nu|\tilde{\Theta}^{l,NF,i}_{k-l\Delta P^{F}_{\alpha\nu},\,\alpha\nu}|GS\rangle = \left(\frac{1}{N_a}\right)^{\frac{\mathcal{N}_{\alpha\nu}-1}{2}} \times e^{-i\mathrm{sgn}(\Delta N^{NF}_{\alpha\nu})[\sum_{j'=0}^{|\Delta N^{NF}_{\alpha\nu}+N^{phNF}_{\alpha\nu}-1} - \sum_{j'=|\Delta N^{NF}_{\alpha\nu}+N^{phNF}_{\alpha\nu}}^{\mathcal{N}_{\alpha\nu}-1}]j'\,a^{0}_{\alpha\nu}\bar{q}_{j'}} \times \delta_{k,l[\Delta P^{F}_{\alpha\nu}+\mathrm{sgn}(\Delta N^{NF}_{\alpha\nu})(\sum_{j'=0}^{\Delta N^{NF}_{\alpha\nu}+N^{phNF}_{\alpha\nu}-1} - \sum_{j'=\Delta N^{NF}_{\alpha\nu}+N^{phNF}_{\alpha\nu}}^{\mathcal{N}_{\alpha\nu}-1})\bar{q}_{j'}]}; \quad \alpha\nu = c0,\, s1,$$

$$\langle f.L;\, \alpha\nu|\tilde{\Theta}^{l,NF,i}_{k-l\Delta P^{0}_{\alpha\nu},\,\alpha\nu}|GS\rangle = \left(\frac{1}{N_a}\right)^{\frac{\mathcal{N}_{\alpha\nu}-1}{2}} e^{-i\sum_{j'=0}^{\mathcal{N}_{\alpha\nu}-1}j'\bar{q}_{j'}} \times \delta_{k,l[\Delta P^{0}_{\alpha\nu}+c_{\alpha\nu}\sum_{j'=0}^{\mathcal{N}_{\alpha\nu}-1}\bar{q}_{j'}]}; \quad \alpha\nu \neq c0,\, s1, \quad (59)$$

for the $\alpha\nu$ pseudofermion spectral functions and

$$\langle f.L;\, p-h,\alpha\nu|\tilde{\Theta}^{l,F,i}_{\alpha\nu}|GS\rangle\,\delta_{k,\,l\Delta P^{phF}_{\alpha\nu}} = \langle 0|F_{J-GS,\,\alpha\nu}\,F_{p-h,\,\alpha\nu}\,F^{\dagger}_{0-GS,\,\alpha\nu}|0\rangle\,\delta_{k,\,l\Delta P^{phF}_{\alpha\nu}};\quad \alpha\nu = c0,\,s1, \quad (60)$$

for the $p-h,\alpha\nu = c0,\,s1$ pseudofermion spectral functions.

The simple form of the matrix elements (59) follows from the full overlap of the generators $F_{J-NF,\,\alpha\nu}$ and $F_{NF,\,\alpha\nu}$ with the operator $\tilde{\Theta}^{l,NF,i}_{k,\,\alpha\nu}$ for the $\alpha\nu = c0,\,s1$ and $\alpha\nu \neq c0,\,s1$ branches, respectively. Such a full overlap also justifies that the corresponding $\alpha\nu$ spectral functions whose expression is given below have a non-interacting character. In turn, the evaluation of the matrix element (60) of the spectral function associated with the $\alpha\nu = c0,\,s1$ pseudofermion elementary processes (B, C) is a more involved problem. For the $\alpha\nu = c0,\,s1$ branches the phase-factor momentum $l\Delta P^{0}_{\alpha\nu} = l[\Delta P^{phF}_{\alpha\nu} + \Delta P^{F}_{\alpha\nu}]$ involves a term, $l\Delta P^{phF}_{\alpha\nu}$, which arises from the elementary processes (C). Interestingly, the dynamics associated with the overlap of the $\alpha\nu = c0,\,s1$ state $\langle f.L;\, p-h,\alpha\nu| = \langle 0|F_{J-GS,\,\alpha\nu}\,F_{p-h,\,\alpha\nu}|$ with the state $\tilde{\Theta}^{l,F,i}_{\alpha\nu}|GS\rangle = \tilde{\Theta}^{l,F,i}_{\alpha\nu}\,F^{\dagger}_{GS,\,\alpha\nu}|0\rangle = F^{\dagger}_{0-GS,\,\alpha\nu}|0\rangle$ of the matrix element (60) is not controlled by the operator $\tilde{\Theta}^{l,NF,i}_{k,\,\alpha\nu}$ but rather results from the different discrete canonical-momentum values of the pseudofermion creation and annihilation operators involved in the generators of each of these states. (For these branches the expression of the operator $\tilde{\Theta}^{l,i}_{k,\,\alpha\nu}$ does not include that of the generator $F^{\dagger}_{p-h,\,\alpha\nu}$, as mentioned above.) Each discrete canonical momentum value of the pseudofermion operators involved in the generators of the former state includes an extra overall canonical-momentum shift $Q_{\alpha\nu}(q)/L$ relative to those of the latter state. If a $\alpha\nu = c0,\,s1$ pseudofermion or pseudofermion hole is created at the *Fermi points* by the elementary processes (B) and thereafter moved from there by the elementary processes (C) generated by the operator $F_{p-h,\,\alpha\nu}$, the dynamics associated with the overlap of the excited-state occupancy configurations generated by the latter processes with the ground-state generator is controlled by the orthogonality catastrophe that occurs in the matrix element (60) due to the overall phase shift $Q_{\alpha\nu}(q)/2$. Such a matrix element involves $N^{0}_{\alpha\nu} + \Delta N^{F}_{\alpha\nu}$ $\alpha\nu$ pseudofermions. The occupancy configuration of the state $F^{\dagger}_{0-GS,\,\alpha\nu}|0\rangle$ corresponds to the densely packed momentum distribution $N^{-0}_{\alpha\nu}(\bar{q}_j)$ for $N^{0}_{\alpha\nu} + \Delta N^{F}_{\alpha\nu}$ $\alpha\nu$ pseudofermions. The corresponding discrete canonical momentum values $\bar{q}_j$ (occupied and unoccupied) are those of the ground state, $\bar{q}_j = q_j$. The occupancy configuration associated with the state $|f.L;\, p-h,\alpha\nu\rangle = F^{\dagger}_{p-h,\,\alpha\nu}\,F^{\dagger}_{J-GS,\,\alpha\nu}|0\rangle$ also refers to $N^{0}_{\alpha\nu} + \Delta N^{F}_{\alpha\nu}$ $\alpha\nu$ pseudofermions. However, its discrete canonical momentum values are those of the excited energy eigenstate. This feature leads to an exotic overlap for the matrix element (60). Such an overlap is behind the unusual quantum-liquid spectral properties, as further discussed below and in reference [3]. We note that in the absence of the $\alpha\nu = c0,\,s1$ pseudofermion overall phase shifts $Q_{\alpha\nu}(q)/2$, Eq. (11), the matrix element (60) would vanish, except for the lowest-peak weight such that $F_{p-h,\,\alpha\nu} = 1$ and thus $\Delta P^{phF}_{\alpha\nu} = 0$.

The spectral function expressions are additive in the contributions of each ground-state–excited-energy-eigenstate transition. For each transition, the available excited-energy-eigenstate pseudofermion discrete canonical-momentum values are in general slightly different and given by the functional (8). The important point is that for each ground-state–excited-state transition one knows the precise values of such discrete pseudofermion canonical momenta. Given these values, the $\alpha\nu$ pseudofermion creation and annihilation operators of the matrix element corresponding to the specific transition act independently for each $\alpha\nu$ excitation branch. This is behind the introduction of the above subspace direct product and follows in part from the factor $\delta_{\alpha\nu,\,\alpha'\nu'}$ on the right-hand side of the pseudofermion anticommutation relation (14). Thus, since the pseudofermion creation and annihilation operators of each $\alpha\nu$ branch act independently for each ground-state–excited-energy-eigenstate transition, they also do it for the whole spectral function, which is additive in the contributions of each ground-state–excited-energy-eigenstate transition. Moreover, as a result of the additive character of the energy in terms of $\alpha\nu$ pseudofermion, independent $-1/2$ holon, and independent $-1/2$ spinon single energies and of the corresponding expression of each J-CPHS ensemble subspace as the direct product of the above considered subspaces, the excited-energy-eigenstate wave-functions of the ground-state normal-ordered 1D Hubbard model factorize. It follows that the spectral functions $B^{l,i}(k,\,\omega)$ of equation (37), generated by transitions from the ground state to a given J-CPHS ensemble subspace, can be expressed as a convolution of pseudofermion spectral functions, one for each branch with finite occupancy in such a subspace and for the independent $-1/2$ holons and/or independent $-1/2$ spinons, if they have finite occupancy in the same subspace, and two functions for the particular case of the $\alpha\nu = c0,\,s1$ branches, as discussed above. It follows from the form of the matrix elements given in equation (60) that the contribution of the corresponding $p-h,\alpha\nu = c0,\,s1$ pseudofermion spectral functions to the weight overlaps is more involved than that of the remaining pseudofermion, independent $-1/2$ holon, and independent $-1/2$ spinon spectral functions.

For each J-CPHS ensemble subspace, we introduce a dimension D associated with the elementary processes (A),

$$D = \sum_{\alpha\nu}\theta(\mathcal{N}_{\alpha\nu}), \quad (61)$$

where the numbers $\mathcal{N}_{\alpha\nu}$ are defined in equation (46). For a general J-CPHS subspace the function $B^{l,i}(k,\,\omega)$ of equation (37) can be written as a convolution of the $p-h,c0,\,s1$ pseudofermion spectral function, $p-h,s1$ pseudofermion spectral function, one $\mathcal{N}_{\alpha\nu}$-$\alpha\nu$ pseudofermion spectral function for each of the D branches such that $\mathcal{N}_{\alpha\nu} > 0$, independent $-1/2$ holon spectral function, and independent

$-1/2$ spinon spectral function. Thus, let us provide the general expressions of the spectral functions corresponding to such a general J-CPHS ensemble subspace.

The $p-h, \alpha\nu = c0, s1$ pseudofermion spectral function associated with the elementary processes (B, C) is given by,

$$B^{l,i}_{Q_{\alpha\nu}}(k,\omega) = \sum_{J-CPHS-\alpha\nu-(C)} |\langle 0|F_{J-GS,\,\alpha\nu}\, F_{p-h,\,\alpha\nu}\, F^{\dagger}_{0-GS,\,\alpha\nu}|0\rangle|^2 \times \delta(\omega - l\Delta E^{phF}_{\alpha\nu})\, \delta_{k,\,l\Delta P^{phF}_{\alpha\nu}};$$
$$\alpha\nu = c0,\, s1 \quad l = \pm 1\,, \quad i = 0, 1, 2, ..., \qquad (62)$$

where the energy and momentum spectra are given below and the matrix element is that of equation (60). The summation $\sum_{J-CPHS-\alpha\nu-(C)}$ runs over the J-CPHS ensemble subspace $\alpha\nu = c0, s1$ pseudofermion occupancy configurations generated by the elementary processes (C). The indices Q_{c0} and Q_{s1} remind us that the overall phase shifts of equation (11) have a specific value for each ground-state–excited-energy-eigenstate transition.

In turn, it follows from the form of the matrix elements of equation (59) that the $\alpha\nu$ pseudofermion spectral function $B^{l,NF,i}_{\alpha\nu}(k,\omega)$ associated with the elementary processes (A) has a non-interacting character and reads,

$$B^{l,NF,i}_{\alpha\nu}(k,\omega) = \left(\frac{1}{N_a}\right)^{\mathcal{N}_{\alpha\nu}-1} \sum_{J-CPHS-\alpha\nu-(A)} \delta(\omega - l\Delta E_{\alpha\nu}) \times \delta_{k,\,l\Delta P_{\alpha\nu}}; \quad l = \pm 1, \quad i = 0, 1, 2, ..., \qquad (63)$$

both for the $\alpha\nu = c0, s1$ and $\alpha\nu \neq c0, s1$ branches. Here the summation $\sum_{J-CPHS-\alpha\nu-(A)}$ runs over the J-CPHS ensemble subspace $\alpha\nu$ pseudofermion occupancy configurations generated by the elementary processes (A). For the $\alpha\nu \neq c0, s1$ branches and densities in the domains $0 < n < 1$ and $0 < m < n$ the number of the latter occupancy configurations is given by $D_{\alpha\nu} = \binom{N^{*}_{\alpha\nu} - N^{F}_{\alpha\nu}}{N^{NF}_{\alpha\nu}}$ and thus can be written as follows,

$$D_{c\nu} = \binom{N_a - N + 2\sum_{\nu'=\nu+1}^{\infty}(\nu'-\nu)N_{c\nu'} + 2L_{c,\,-1/2} - N^{F}_{c\nu}}{N^{NF}_{c\nu}}; \quad \nu > 0,$$
$$D_{s\nu} = \binom{N_{\uparrow} - N_{\downarrow} + 2\sum_{\nu'=\nu+1}^{\infty}(\nu'-\nu)\Delta N_{c\nu'} + 2L_{c,\,-1/2} - N^{F}_{s\nu}}{N^{NF}_{s\nu}}; \quad \nu > 1, \qquad (64)$$

where the values of N, $N_{\uparrow}$, and $N_{\downarrow}$ are those of the corresponding excited-state CPHS ensemble subspace. We recall that for the $c\nu \neq c0$ (and $s\nu \neq s1$) branches and electronic density $n = 1$ (and spin density $m = 0$) the spectral function $B^{l,NF,i}_{c\nu}(k,\omega)$ (and $B^{l,NF,i}_{s\nu}(k,\omega)$) of equation (63) does not exist.

Finally, the form of the operator $\tilde{\Theta}^{l,F,i}_{\alpha\nu}$ implies that $\langle GS|F_{F,\,\alpha\nu}\tilde{\Theta}^{l,F,i}_{\alpha\nu}|GS\rangle = 1$ for the $\alpha\nu \neq c0, s1$ branches with finite occupancy in the J-CPHS ensemble subspace. This together with the non-interacting character of the $-1/2$ Yang holons and $-1/2$ HL spinons is behind the form of the independent $-1/2$ holon ($\alpha = c$) and independent $-1/2$ spinon ($\alpha = s$) spectral function, which reads,

$$B^{l,i}_{\alpha,\,-1/2}(k,\omega) = \frac{1}{\mathcal{C}_{\alpha}}\,\delta(\omega - lE_{\alpha})\,\delta_{k,\,lP_{\alpha}}; \quad \alpha = c,\, s. \qquad (65)$$

Here the coefficient $\mathcal{C}_{\alpha}$ is given in equation (24). While all spectral functions provided in equations (63) and (65) have a non-interacting character, the $p-h, c0$ and $p-h, s1$ pseudofermion spectral functions of equation (62) correspond to a more complex problem. The latter functions are further studied in reference [3] for the metallic phase.

The $\alpha\nu$ pseudofermion energy spectrum $\Delta E_{\alpha\nu}$ on the right-hand side of equations (62) and (63) can be expressed in terms of the bare-momentum distribution function deviations. The energy spectra $\Delta E_{\alpha\nu}$ and $\Delta E^{phF}_{\alpha\nu}$ appearing in the latter equations and in equation (62), respectively, and the the independent $-1/2$ holon ($\alpha = c$) and independent $-1/2$ spinon ($\alpha = s$) energy E_{α} of equation (65) read,

$$\Delta E_{\alpha\nu} = \sum_{q_j=-q^{0}_{\alpha\nu}}^{+q^{0}_{\alpha\nu}} \Delta N^{NF}_{\alpha\nu}(q_j)\,\epsilon_{\alpha\nu}(q_j);$$
$$\Delta E^{phF}_{\alpha\nu} = \frac{2\pi}{L}\, v_{\alpha\nu}\,[m_{\alpha\nu,\,+1} + m_{\alpha\nu,\,-1}]; \quad \alpha\nu = c0,\, s1;$$
$$E_{\alpha} = \mu_{\alpha}\left[L_{\alpha,\,-1/2} + \delta_{\alpha,\,c}\,N^{F}_{c1} + \sum_{\nu=2}^{\infty}\nu N^{F}_{\alpha\nu}\right];$$
$$\alpha = c,\, s; \quad \mu_c = 2\mu, \quad \mu_s = 2\mu_0\, H. \qquad (66)$$

The momentum spectra corresponding to such energy spectra are given by,

$$\Delta P_{\alpha\nu} = \sum_{q_j=-q^{0}_{\alpha\nu}}^{+q^{0}_{\alpha\nu}} \Delta N^{NF}_{\alpha\nu}(q_j)\,q_j + \Delta P^{F}_{\alpha\nu};$$
$$\Delta P^{phF}_{\alpha\nu} = \frac{2\pi}{L}\,[m_{\alpha\nu,\,+1} - m_{\alpha\nu,\,-1}]; \quad \alpha\nu = c0,\, s1;$$
$$\Delta P^{F}_{c0} = 4k_F\Big[\Delta J^{F}_{c0} + \sum_{\nu=1}^{\infty} J^{I}_{c\nu} + \sum_{\nu=2}^{\infty} J^{I}_{s\nu}\Big];$$
$$\Delta P^{F}_{s1} = 2k_{F\downarrow}\Big[\Delta J^{F}_{s1} - 2\sum_{\nu=2}^{\infty} J^{I}_{s\nu}\Big];\ 0 < n < 1,\ 0 < m < n;$$
$$\Delta P_{c\nu} = \sum_{q_j=-q^{0}_{c\nu}}^{+q^{0}_{c\nu}} \Delta N^{NF}_{c\nu}(q_j)\,[(1+\nu)\pi - q_j];$$
$$\Delta P_{s\nu} = \sum_{q_j=-q^{0}_{\alpha\nu}}^{+q^{0}_{\alpha\nu}} \Delta N^{NF}_{\alpha\nu}(q_j)\,q_j\,; \quad \alpha\nu \neq c0,\, s1;$$
$$P_c = \pi\,[L_{c,\,-1/2} + \sum_{\nu=1}^{\infty}\nu N^{F}_{c\nu}]; \quad P_s = 0. \qquad (67)$$

In these equations $\epsilon_{c\nu}(q_j) = 2\nu\mu + \epsilon^{0}_{c\nu}(q_j)$ for $\nu > 0$, $\epsilon_{s\nu}(q_j) = 2\nu\mu_0\, H + \epsilon^{0}_{s\nu}(q_j)$ for $\nu > 1$, the bands $\epsilon_{\alpha\nu}(q_j)$

for $\alpha\nu = c0,\, s1$ and $\epsilon^0_{\alpha\nu}(q_j)$ for $\alpha\nu \neq c0,\, s1$ are defined by equations (C.15)–(C.21) of reference [9], the small energy $\Delta E^{phF}_{\alpha\nu}$ is such that $m_{\alpha\nu,\,\pm 1}$ is the number of elementary $\alpha\nu = c0,\, s1$ pseudofermion particle-hole processes (C) considered above, $v_{\alpha\nu} \equiv v_{\alpha\nu}(q^0_{F\alpha\nu})$, and $v_{\alpha\nu}(q) = \partial\epsilon_{\alpha\nu}(q)/\partial q$.

As further discussed in reference [3], for densities $0 < n < 1$ and $0 < m < n$ the elementary processes (C) leading to the spectral-function singular features include contributions from small but finite values of $m_{\alpha\nu,\,\pm 1}/N_a$ as $N_a \rightarrow \infty$. For $n = 1$ (and $m = 0$) the latter processes do not exist for the $c0$ (and $s1$) branch and thus $\Delta E^{phF}_{c0} = 0$ and $\Delta P^{phF}_{c0} = 0$ (and $\Delta E^{phF}_{s1} = 0$ and $\Delta P^{phF}_{s1} = 0$).

Let us consider the general situation when the J-CPHS ensemble subspace has finite occupancy for the $c0$ and $s1$ pseudofermion branches, $D - 2 > 0$ $\alpha\nu \neq c0,\, s1$ pseudofermion branches, independent $-1/2$ holons, and independent $-1/2$ spinons. In this case the functions $B^{l,i}(k,\,\omega)$ of equation (37) can be written as,

$$
\begin{aligned}
B^{l,i}(k,\,\omega) &= \frac{1}{G_C}\, G^{l,i}(k,\,\omega) \\
&= \left(\prod_{\alpha=c,\,s}\frac{1}{C_\alpha}\right)\left(\prod_{j=1}^{D}\left(\frac{1}{N_a}\right)^{\mathcal{N}_{\alpha\nu_j}}\left[\sum_{J-CPHS-\alpha\nu_j-(A)}\right]\right) \\
&\times \frac{1}{N_a}\sum_{k'}\sum_{\omega'} B^{l,i}_{Q_{s1}}\left(k',\omega'\right) \times B^{l,i}_{Q_{c0}}\left(k - l\sum_{j=1}^{D}\Delta P_{\alpha\nu_j}\right. \\
&\left. - l\sum_{\alpha=c,\,s} P_\alpha - k', \omega - l\sum_{j=1}^{D}\Delta E_{\alpha\nu_j} - l\sum_{\alpha=c,\,s} E_\alpha - \omega'\right); \\
G_C &= \left(\prod_{\alpha=c,\,s}\mathcal{C}_\alpha\right)\left[\sum_J\sum_k\int_0^{l\infty} d\omega\, G^{l,i}(k,\,\omega)\right]\Bigg/ \\
&\left[\sum_f\sum_{j=1}^{N_a}|\langle f.L\,;C|\tilde{\Theta}^l_{\mathcal{N}_i,\,j}|GS\rangle|^2\right]; \\
C_c &\equiv \mathcal{C}_c; \quad C_s \equiv G_C\,\mathcal{C}_s; \quad i = 0,1,2,...; \quad l = \pm 1, \quad (68)
\end{aligned}
$$

where

$$
\begin{aligned}
G^{l,i}(k,\,\omega) &= \sum_{k_1}\sum_{\omega_1} B^{l,i}_{Q_{c0}}(k - k_1, \omega - \omega_1) \\
&\times \left[\prod_{j=1}^{D}\frac{1}{N_a}\sum_{k_{j+1}}\sum_{\omega_{j+1}} B^{l,NF,i}_{\alpha\nu_j}(k_j - k_{j+1}, \omega_j - \omega_{j+1})\right] \\
&\times \left[\prod_{j=D+1}^{D+2} B^{l,i}_{\alpha_j,\,-1/2}(k_j - k_{j+1}, \omega_j - \omega_{j+1})\right] \\
&\times \frac{1}{N_a} B^{l,i}_{Q_{s1}}(k_{D+3}, \omega_{D+3}),
\end{aligned}
$$

the coefficient G_C, which also appears in the quantity $C_J = e^{i\,j\Delta P_J}\,[G_C/G_J]$ given in equation (46) and in the operator expression of equation (57), has a uniquely defined value for each CPHS ensemble subspace, $\tilde{\Theta}^l_{\mathcal{N}_i,\,j}$ is the corresponding operator on the right-hand side of equation (32), the summation $\sum_f$ runs over all energy eigenstates of the CPHS ensemble subspace, and the summation $\sum_J$ is over all J-CPHS ensemble subspaces of that subspace. Moreover, the pseudofermion spectral functions appearing in the $G^{l,i}(k,\,\omega)$ expression are given in equations (62) and (63), the independent $-1/2$ holon and $-1/2$ spinon spectral functions are provided in equation (65), $\alpha_{D+1} = c$ and $\alpha_{D+2} = s$ labels the independent $-1/2$ holons and independent $-1/2$ spinons, respectively, the momenta $k_1, k_2, ..., k_{D+3}$ and energies $\omega_1, \omega_2, ..., \omega_{D+3}$ correspond to summation variables, and the index $\alpha\nu_j$, where $j = 1, ..., D$, is such that $\alpha\nu_1 = c0$, $\alpha\nu_2 = s1$, and for $j = 3, ..., D$ $\alpha\nu_j$ refers to the $D - 2$ $\alpha\nu \neq c0,\, s1$ pseudofermion branches such that $N^{NF}_{\alpha\nu} > 0$ for the J-CPHS ensemble subspace. To reach the second expression of equation (68) from the expression for $G^{l,i}(k,\,\omega)/G_C$, we used the non-interacting form of the spectral functions given in equations (63) and (65) to perform $D + 2$ momentum and energy summations. It follows that the general spectral function $B^{l,i}(k,\,\omega)$ of equation (37) can be written as a convolution of the $p-h, c0$ and $p-h, s1$ pseudofermion spectral functions alone, as given in the second expression of equation (68). We recall that for the $i = 0$ function $B^{l,0}(k,\,\omega)$ the value of the coefficient G_C is independent of U/t and for the dominant CPHS ensemble subspaces considered in Section 4 corresponding to that function, it reads $G_C = 1$ for all values of U/t.

For J-CPHS subspaces with no finite pseudofermion occupancy for the $\alpha\nu \neq c0,\, s1$ pseudofermion branches and/or no independent $-1/2$ holon and/or independent $-1/2$ spinon occupancy, the spectral function $B^{l,i}(k,\,\omega)$ has the same general form as in equation (68), except for the absence in the expression of $G^{l,i}(k,\,\omega)$ of the spectral functions corresponding to the missing branches and/or quantum object types. Note also that the expression for $G^{l,i}(k,\,\omega)$ and thus for $B^{l,i}(k,\,\omega) = G^{l,i}(k,\,\omega)/G_C$ given in the unnumbered equation after equation (68) is valid for electronic density $n = 1$ (and spin density $m = 0$), provided that for $j = 3, ..., D$ the index $\alpha\nu_j$ refers to the $D - 2$ $s\nu \neq s1$ (and $c\nu \neq c0$) pseudofermion branches such that $N^{NF}_{\alpha\nu} > 0$ for the J-CPHS ensemble subspace. Moreover, for $n = 1$ (and $m = 0$) one must use $c0$ (and $s1$) pseudofermion spectral functions specific to the corresponding excitation spectrum. These functions are studied elsewhere. However, the second expression of equation (68) refers to densities in the domains $0 < n < 1$ and $0 < m < n$ only.

The probability amplitudes $|\langle 0|F_{0-GS,\,\alpha\nu}\times F^\dagger_{p-h,\,\alpha\nu}\,F^\dagger_{J-GS,\,\alpha\nu}|0\rangle|^2$ associated with the matrix element (60) which appear in expression (62) have the following general form,

$$
\begin{aligned}
&\left|\langle 0|F_{0-GS,\,\alpha\nu}\,F^\dagger_{p-h,\,\alpha\nu}\,F^\dagger_{J-GS,\,\alpha\nu}|0\rangle\right|^2 = \\
&\left|\langle 0|f_{q'_{N^0_{\alpha\nu}+\Delta N^F_{\alpha\nu}},\alpha\nu}\cdots f_{q'_1,\,\alpha\nu} f^\dagger_{\bar{q}_1,\alpha\nu}\cdots f^\dagger_{\bar{q}_{N^0_{\alpha\nu}+\Delta N^F_{\alpha\nu}},\alpha\nu}|0\rangle\right|^2, \quad (69)
\end{aligned}
$$

where $\alpha\nu = c0,\, s1$. In expression (69) we have considered that the ground state corresponds to pseudofermion annihilation operators and the pseudofermion operators left for

$$\left|\left| \begin{array}{lll} \{f^{\dagger}_{\bar{q}_1,\,\alpha\nu}\,,f_{q'_1,\,\alpha\nu}\} & \{f^{\dagger}_{\bar{q}_1,\,\alpha\nu}\,,f_{q'_2,\,\alpha\nu}\} & \cdots\{f^{\dagger}_{\bar{q}_1,\,\alpha\nu}\,,f_{q'_{N^0_{\alpha\nu}+\Delta N^F_{\alpha\nu}},\,\alpha\nu}\} \\ \{f^{\dagger}_{\bar{q}_2,\,\alpha\nu},f_{q'_1,\,\alpha\nu}\} & \{f^{\dagger}_{\bar{q}_2,\,\alpha\nu}\,,f_{q'_2,\,\alpha\nu}\} & \cdots\{f^{\dagger}_{\bar{q}_2,\,\alpha\nu}\,,f_{q'_{N^0_{\alpha\nu}+\Delta N^F_{\alpha\nu}},\,\alpha\nu}\} \\ \cdots\cdots & \cdots\cdots & \cdots\cdots \\ \{f^{\dagger}_{\bar{q}_{N^0_{\alpha\nu}+\Delta N^F_{\alpha\nu}},\,\alpha\nu}\,,f_{q'_1,\,\alpha\nu}\} & \{f^{\dagger}_{\bar{q}_{N^0_{\alpha\nu}+\Delta N^F_{\alpha\nu}},\,\alpha\nu}\,,f_{q'_2,\,\alpha\nu}\} & \cdots\{f^{\dagger}_{\bar{q}_{N^0_{\alpha\nu}+\Delta N^F_{\alpha\nu}},\,\alpha\nu}\,,f_{q'_{N^0_{\alpha\nu}+\Delta N^F_{\alpha\nu}},\,\alpha\nu}\} \end{array} \right|\right|^2 , \tag{70}$$

$$\left(\frac{1}{N^*_{\alpha\nu}}\right)^{2[N^0_{\alpha\nu}+\Delta N^F_{\alpha\nu}]} \Big[\prod_{j=1}^{N^*_{\alpha\nu}} \sin^2\Big(\frac{N^{ph}_{\alpha\nu}(q_j)\,[Q_{\alpha\nu}(q_j)-\pi]+\pi}{2}\Big)\Big]$$

$$\times \left|\left| \begin{array}{lll} \frac{1}{\sin\left(\frac{\bar{q}_1-q'_1}{2}\right)} & \frac{1}{\sin\left(\frac{\bar{q}_1-q'_2}{2}\right)} & \cdots\frac{1}{\sin\left(\frac{\bar{q}_1-q'_{N^0_{\alpha\nu}+\Delta N^F_{\alpha\nu}}}{2}\right)} \\ \frac{1}{\sin\left(\frac{\bar{q}_2-q'_1}{2}\right)} & \frac{1}{\sin\left(\frac{\bar{q}_2-q'_2}{2}\right)} & \cdots\frac{1}{\sin\left(\frac{\bar{q}_2-q'_{N^0_{\alpha\nu}+\Delta N^F_{\alpha\nu}}}{2}\right)} \\ \cdots\cdots & \cdots\cdots & \cdots\cdots \\ \frac{1}{\sin\left(\frac{\bar{q}_{N^0_{\alpha\nu}+\Delta N^F_{\alpha\nu}}-q'_1}{2}\right)} & \frac{1}{\sin\left(\frac{\bar{q}_{N^0_{\alpha\nu}+\Delta N^F_{\alpha\nu}}-q'_2}{2}\right)} & \cdots\frac{1}{\sin\left(\frac{\bar{q}_{N^0_{\alpha\nu}+\Delta N^F_{\alpha\nu}}-q'_{N^0_{\alpha\nu}+\Delta N^F_{\alpha\nu}}}{2}\right)} \end{array} \right|\right|^2 , \tag{71}$$

the excited energy eigenstate are of creation character. At this stage, for the evaluation of $\mathcal{N}$-electron spectral functions, the main problem remaining is the computation of the non-trivial probability amplitude (69), which can be expressed by the following determinant,

see equation (70) above

for the $\alpha\nu = c0,\, s1$ branches. This result is justified by the following pseudofermion properties. First, the pseudofermions have no residual-interaction energy terms, as discussed in references [3,20]. Second, the canonical-momentum shift $Q_{\alpha\nu}(q_j)/L$, which under the ground-state–excited-energy-eigenstate transition involves all $\alpha\nu = c0,\, s1$ pseudofermions of the initial ground state, is a zero-energy process [10]. Third, the elementary pseudofermion processes (C) correspond to $\alpha\nu = c0,\, s1$ pseudoparticle particle-hole processes whose energy spectrum is of non-interacting character for the pseudoparticles, what implies that the energy spectrum $\Delta E^{phF}_{\alpha\nu} = [2\pi/L]\, v_{\alpha\nu}\, m_{\alpha\nu}$ of equation (66) remains linear in $m_{\alpha\nu}$ for small finite values of $m_{\alpha\nu}/N_a$ as $N_a \rightarrow \infty$ [3,20].

In spite of the non-interacting form of the determinant (70), the unusual pseudofermion anticommutation relations (14) give rise to unusual physics, in the form of an orthogonality catastrophe. (The absence of such an orthogonality catastrophe would require that $Q_{\alpha\nu}(q)/2 = 0$.) Indeed, replacement of the anticommutator (14) in the determinant (70) leads to,

see equation (71) above

for the $\alpha\nu = c0,\, s1$ branches, where the overall phase shift $Q_{\alpha\nu}(q_j)/2$ is given in equation (11) and the bare-momentum distribution function $N^{ph}_{\alpha\nu}(q_j)$ is such that $N^{ph}_{\alpha\nu}(q_j) = \mathcal{N}^{ph}_{\alpha\nu}(\bar{q}_j)$. Here $\mathcal{N}^{ph}_{\alpha\nu}(\bar{q}_j)$ is the pseudofermion canonical-momentum distribution function given in equation (56), which includes the low-energy and small-momentum $\alpha\nu = c0,\, s1$ pseudofermion particle-hole processes (C). The determinant of Eq. (71) can be rewritten as,

$$\left(\frac{1}{N^*_{\alpha\nu}}\right)^{2[N^0_{\alpha\nu}+\Delta N^F_{\alpha\nu}]} \prod_{j=1}^{N^*_{\alpha\nu}} \sin^2\left(\frac{N^{ph}_{\alpha\nu}(q_j)\,[Q_{\alpha\nu}(q_j)-\pi]+\pi}{2}\right)$$
$$\times \prod_{j=1}^{N^*_{\alpha\nu}} \prod_{i=1}^{N^*_{\alpha\nu}} \theta(i-j) \sin^2\left(\frac{N^{-0}_{\alpha\nu}(q'_j)N^{-0}_{\alpha\nu}(q'_i)[q'_j-q'_i-\pi]+\pi}{2}\right)$$
$$\times \prod_{j=1}^{N^*_{\alpha\nu}} \prod_{i=1}^{N^*_{\alpha\nu}} \theta(i-j)\, \sin^2\left(\frac{N^{ph}_{\alpha\nu}(q_j)N^{ph}_{\alpha\nu}(q_i)[\bar{q}_j-\bar{q}_i-\pi]+\pi}{2}\right)$$
$$\times \prod_{j=1}^{N^*_{\alpha\nu}} \prod_{i=1}^{N^*_{\alpha\nu}} \frac{1}{\sin^2\left(\frac{N^{ph}_{\alpha\nu}(q_i)N^{-0}_{\alpha\nu}(q'_j)[\bar{q}_i-q'_j-\pi]+\pi}{2}\right)};\;\; \alpha\nu = c0,\, s1, \tag{72}$$

where $N^{-0}_{\alpha\nu}(q_j) = \mathcal{N}^{-0}_{\alpha\nu}(\bar{q}_j)$ is a densely packed bare-momentum distribution function whose *Fermi points* are given by $q^0_{F\alpha\nu,\,\pm1} = \pm q^0_{F\alpha\nu} \pm [2\pi/L]\Delta N^{0,F}_{\alpha\nu,\,\pm1}$ and the corresponding canonical-momentum distribution function $\mathcal{N}^{-0}_{\alpha\nu}(\bar{q}_j)$ is that of equation (56) whose *Fermi points* read $\bar{q}_{F\alpha\nu,\,\pm1} = \pm q^0_{F\alpha\nu} \pm [2\pi/L][\Delta N^F_{\alpha\nu,\,\pm1} \pm Q^{\Phi}_{\alpha\nu}(\pm q^0_{F\alpha\nu})/2\pi]$. The expressions (70)–(72) are used in reference [3] in the derivation of finite-energy spectral-weight distributions for the model metallic phase.

6 Discussion and concluding remarks

The main result of this paper is the general spectral function expression defined by equations (36) and (68). The expression given in the latter equation involves the $p-h, c0$ and $p-h, s1$ pseudofermion spectral functions provided in equation (62), whose probability amplitude $|\langle 0|F_{J-GS,\,\alpha\nu}\, F_{p-h,\,\alpha\nu}\, F^{\dagger}_{0-GS,\,\alpha\nu}|0\rangle|^2$ can be expressed in terms of the determinants of equations (70)–(72). An important aspect of the pseudofermion dynamical theory

introduced in this paper and further developed in reference [3] for the metallic phase, is the different origin of the dynamics associated with the matrix-element overlaps of the $\alpha\nu = c0$, $s1$ pseudofermion occupancy configurations in the vicinity and away of the *Fermi points*.

The studies of this paper considered the 1D Hubbard model, which describes successfully some of the exotic properties observed in low-dimensional materials [1,2,17,23]. Our results also apply to related integrable interacting problems [24] and therefore have wide applicability. In reference [2] the finite-energy spectral function expressions derived by use of the pseudofermion dynamical theory introduced here are applied to the study of the spectral-weight features observed in the quasi-1D organic compound TTF-TCNQ. Interestingly, one finds quantitative agreement with the observed spectral features for the whole experimental energy band width. The microscopic mechanisms found in reference [1] by use of our theory are also consistent with the phase diagram observed in the $(TMTTF)_2X$ and $(TMTSF)_2X$ series of organic compounds and explain the absence of superconducting phases in TTF-TCNQ. Our theory is also of interest for the understanding of the spectral properties of the new quantum systems described by ultra-cold fermionic atoms on an optical lattice [7].

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