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# Scattering mechanisms and spectral properties of the one-dimensional Hubbard model

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**Abstract**

It is found that the finite-energy spectral properties of the one-dimensional Hubbard model are controlled by the scattering of charged $\eta$-spin-zero $2\nu$-holon composite objects, spin-zero $2\nu$-spinon composite objects, and charged $\eta$-spinless and spinless objects, rather than by the scattering of independent $\eta$-spin-1/2 holons and spin-1/2 spinons. Here $\nu = 1, 2, \ldots$. The corresponding $S$ matrix is calculated and its relation to the spectral properties is clarified.

The description of the microscopic scattering mechanisms behind the unusual finite-energy spectral properties observed in low dimensional materials has remained until now an interesting open problem. The one-dimensional (1D) Hubbard Hamiltonian is the simplest model for the description of electronic correlations in a chain of $N_a$ sites. It reads $\hat{H} = \hat{T} + U\hat{D} - [U/2][\hat{N} - N_a/2]$, where $\hat{T} = -t\sum_{\sigma=\uparrow,\downarrow}\sum_{j=1}^{N_a}[c^{\dagger}_{j,\sigma}c_{j+1,\sigma} + \text{h.c.}]$ is the *kinetic energy* operator, $\hat{D} = \sum_j \hat{n}_{j,\uparrow}\hat{n}_{j,\downarrow}$ the electron double-occupation operator, $\hat{N} = \sum_{j,\sigma}\hat{n}_{j,\sigma}$ the electron number operator, and the operator $c^{\dagger}_{j,\sigma}$ creates a spin-$\sigma$ electron at site $j$. In contrast to other interacting models [1] and in spite of the model exact solution [2], until recently little was known about its finite-energy spectral properties for finite values of the on-site repulsion $U$. Recently, the problem was studied using the pseudofermion dynamical theory (PDT) introduced in [3, 4], whose predictions agree quantitatively for the whole momentum and energy bandwidth with the peak dispersions observed for the TCNQ stacks by angle-resolved photoelectron spectroscopy for the quasi-1D conductor TTF-TCNQ and are consistent with the phase diagram observed for the $(TMTTF)_2X$ and $(TMTSF)_2X$ series of compounds [5]. More recently, results for the TTF-TCNQ spectrum consistent with those from the PDT were obtained by the dynamical density matrix renormalization group method [6]. Within the PDT, the finite-energy spectral properties are controlled by the functional character of the pseudofermion anticommutators [4, 5]. However, the relation of these anticommutators to the elementary-excitation $S$ matrix remains an open question. Moreover, the fact that these anticommutators do not couple quantum objects with different $\eta$-spin or spin projections seems

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to be inconsistent with the form of the $S$ matrix for elementary excitations calculated in [7, 8]. Thus, the study of the relation of the PDT to the elementary-excitation scattering is an important issue both for the clarification of that apparent inconsistency and the further understanding of the scattering mechanisms that control the exotic finite-energy spectral properties of low dimensional materials and of the new quantum systems described in terms of cold fermionic atoms on an optical lattice [5, 9].

In this paper the above problems are solved by identifying the active scatterers and scattering centres which control the dynamical properties, calculating their $S$ matrix, and clarifying its relation to the spectral properties. Moreover, the connection to the $S$ matrix of [7, 8] is also clarified. The number of lattice sites $N_a$ is considered large, units of Planck constant and lattice spacing one are used, and the lattice length is denoted by $L = N_a$ and the electronic charge by $-e$. The densities $n = N/L$ and spin densities $m = [N_\uparrow - N_\downarrow]/L$ are in the domains $0 < n \leqslant 1$ and $0 \leqslant m < n$, respectively. The above Hamiltonian commutes with the generators of the $\eta$-spin and spin $SU(2)$ algebras [10]. Here the $\eta$-spin and spin values of an energy eigenstate are called $\eta$ and $S$, respectively, and the corresponding projections $\eta_z$ and $S_z$. A key result needed for our study is that all energy eigenstates of the model can be described in terms of occupancy configurations of $\eta$-spin-$1/2$ holons, spin-$1/2$, spinons, and $\eta$-spinless and spinless $c0$ pseudoparticles [10]. Below, the notation $\pm 1/2$ holons and $\pm 1/2$ spinons is used according to the values of the $\eta$-spin and spin projections, respectively. The electron–rotated-electron unitary transformation [10] maps the electrons onto rotated electrons such that rotated-electron double occupation, no occupation, and spin-up and spin-down single occupation are good quantum numbers for all values of $U$. The $\pm 1/2$ holons of charge $\pm 2e$ and zero spin and the chargeless $\pm 1/2$ spinons are generated from the electrons by that unitary transformation. The corresponding holon and spinon number operators $\hat{M}_{c,\pm 1/2}$ and $\hat{M}_{s,\pm 1/2}$, respectively, are of the form given in equation (24) of [10] and involve the electron–rotated-electron unitary operator. While the $-1/2$ and $+1/2$ holons refer to the rotated-electron doubly occupied and unoccupied sites, respectively, the $-1/2$ and $+1/2$ spinons correspond to the spin degrees of freedom of the spin-down and spin-up rotated-electron singly occupied sites, respectively. The charge degrees of freedom of the latter sites are described by the spinless and $\eta$-spinless $c0$ pseudoparticles, which are composite objects made up of a charge $-e$ chargeon and a charge $+e$ antichargeon [10]. The $c\nu$ pseudoparticles (and $s\nu$ pseudoparticles) such that $\nu = 1, 2, \ldots$ are $\eta$-spin singlet (and spin singlet) $2\nu$-holon (and $2\nu$-spinon) composite objects. Thus, $M_{\alpha,\pm 1/2} = L_{\alpha,\pm 1/2} + \sum_{\nu=1}^{\infty} \nu N_{\alpha\nu}$ where $\alpha = c, s$, $N_{\alpha\nu}$ denotes the number of $\alpha\nu$ pseudoparticles, and $L_{c,\pm 1/2} = \eta \mp \eta_z$ and $L_{s,\pm 1/2} = S \mp S_z$ give the numbers of $\pm 1/2$ Yang holons and $\pm 1/2$ HL spinons, respectively. Those are the holons and spinons that are not part of composite pseudoparticles. All energy eigenstates can be described by occupancy configurations of $\alpha\nu$ pseudoparticles, $-1/2$ Yang holons, and $-1/2$ HL spinons [10]. For the ground state, $N_{c0} = N$, $N_{s1} = N_\downarrow$, $N_{\alpha\nu} = L_{c,-1/2} = L_{s,-1/2} = 0$ for $\alpha\nu \neq c0, s1$.

In our study we consider the *pseudofermion subspace* (PS), which is spanned by the initial ground state $|GS\rangle$ and all excited energy eigenstates contained in $\hat{O}|GS\rangle$, where $\hat{O}$ is any one-electron or two-electron operator. In reference [3] it is shown that within the PS there is a unitary transformation that maps the $\alpha\nu$ *pseudoparticle* or hole onto the $\alpha\nu$ *pseudofermion* or hole, respectively. These objects differ only in the discrete momentum values. The $\alpha\nu$ pseudoparticle or hole has discrete bare-momentum values $q_j = [2\pi/L]I_j^{\alpha\nu}$ such that $I_j^{\alpha\nu}$ are consecutive integers or half-odd integers [10]. These values are good quantum numbers whose allowed occupancies are one (pseudoparticle) and zero (hole) only. The $\alpha\nu$ pseudofermion or hole has discrete canonical-momentum values given by

$$\bar{q}_j = \bar{q}(q_j) = q_j + Q^{\Phi}_{\alpha\nu}(q_j)/L, \tag{1}$$

where $j = 1, 2, \ldots, N^*_{\alpha\nu}$, $N^*_{\alpha\nu} = N_{\alpha\nu} + N^h_{\alpha\nu}$, and $N^h_{\alpha\nu}$ denotes the number of $\alpha\nu$ pseudofermion holes, which equals that of $\alpha\nu$ pseudoparticle holes, whose value is given in equation (B.11) of [10]. Such a canonical-momentum pseudofermion is related in [3] to the *local* $\alpha\nu$ *pseudofermion* by a suitable Fourier transformation. The latter object occupies the sites of the effective $\alpha\nu$ lattice [3, 4]. Except for the discrete momentum values, the above pseudoparticle and pseudofermion have the same properties. Thus, all the energy eigenstates that span the PS can be described by occupancy configurations of $\alpha\nu$ pseudofermions, $-1/2$ Yang holons, and $-1/2$ HL spinons [3, 4]. The functional,

$$Q^{\Phi}_{\alpha\nu}(q_j) = 2\pi \sum_{\alpha'\nu', j} \Phi_{\alpha\nu,\alpha'\nu'}(q_j, q_{j'})\Delta N_{\alpha'\nu'}(q_{j'}), \tag{2}$$

of equation (1) was introduced in [3] and is such that $Q^{\Phi}_{\alpha\nu}(q_j)/2$ is found below to be an overall scattering phase shift. Here $\Delta N_{\alpha\nu}(q_j) \equiv N_{\alpha\nu}(q_j) - N^0_{\alpha\nu}(q_j)$ is the $\alpha\nu$ branch bare-momentum distribution-function deviation relative to the ground-state value and $\pi\,\Phi_{\alpha\nu,\alpha'\nu'}(q, q')$ is defined in [3] and is found below to be an elementary *two-pseudofermion phase shift*. Note that $Q^{\Phi}_{\alpha\nu}(q_j) = 0$ for the initial ground state and thus $\bar{q}_j = q_j$ for that state.

Each transition from the initial ground state to a PS excited energy eigenstate can be divided into two elementary processes. The first process is a scattering-less finite-energy and finite-momentum excitation which transforms the ground state onto a well defined virtual state. This excitation involves the pseudofermion creation, annihilation, and particle–hole processes associated with the PS excited state and the discrete bare-momentum shift $Q^0_{\alpha\nu}/L$, whose possible values are $0, \pm\pi/L$ [3], for $\alpha\nu$ branches with finite occupancy in that state. For $\nu > 0$ branches that excitation can involve a change in the number of discrete bare-momentum values. Although the $\alpha\nu \neq c0, s1$ branches have no finite pseudofermion occupancy in the initial ground state, one can define the values $N^*_{\alpha\nu} = N^h_{\alpha\nu}$ for the corresponding empty bands [10, 3, 4]. In this first step the pseudofermions acquire the excitation momentum and energy needed for the second-step scattering events. Thus, the virtual state is the in asymptote of the pseudofermion scattering theory. The second elementary step of the ground-state transition involves a set of elementary scattering events where all $\alpha\nu$ pseudofermions or holes of momentum $q_j + Q^0_{\alpha\nu}/L$ of the in asymptote are the scatterers. Each of these elementary scattering events leads to a phase factor in the wavefunction of the $\alpha\nu$ pseudofermions or holes given by

$$S_{\alpha\nu,\alpha'\nu'}(q_j, q_{j'}) = \mathrm{e}^{\mathrm{i}2\pi\,\Phi_{\alpha\nu,\alpha'\nu'}(q_j,q_{j'})\Delta N_{\alpha'\nu'}(q_{j'})}. \tag{3}$$

The scattering centres are the $\alpha'\nu'$ pseudofermions or holes of momentum $q_{j'} + Q^0_{\alpha\nu}/L$ created in the ground-state–virtual-state transition and thus such that $\Delta N_{\alpha'\nu'}(q_{j'}) \neq 0$. Indeed, note that $S_{\alpha\nu,\alpha'\nu'}(q_j, q_{j'}) = 1$ for $\Delta N_{\alpha'\nu'}(q_{j'}) = 0$. There is a one-to-one correspondence between the local rotated-electron occupancy configurations that describe the PS energy eigenstates and the local $\alpha\nu$ pseudofermion occupancy configurations and $-1/2$ Yang holon and $-1/2$ HL spinon occupancies that describe the same states [4]. The corresponding effective $\alpha\nu$ lattices have the same length $L$ as the original lattice. Our analysis refers to periodic boundary conditions and the thermodynamic limit $L \to \infty$. Under a ground-state–excited-energy-eigenstate transition, by moving the $\alpha\nu$ pseudofermion or hole of initial ground-state momentum $q_j$ once around the length-$L$ lattice ring, its wavefunction acquires the following overall phase factor:

$$S_{\alpha\nu}(q_j) = \mathrm{e}^{\mathrm{i}Q^0_{\alpha\nu}} \prod_{\alpha'\nu'} \prod_{j'=1}^{N^*_{\alpha'\nu'}} S_{\alpha\nu,\alpha'\nu'}(q_j, q_{j'}) = \mathrm{e}^{\mathrm{i}Q_{\alpha\nu}(q_j)}; \qquad j = 1, 2, \ldots, N^*_{\alpha\nu}. \tag{4}$$

Interestingly, $Q_{\alpha\nu}(q_j)/L$ is the net $\alpha\nu$ pseudofermion or hole discrete canonical-momentum shift that arises due to the above transition [3, 4] and thus, in this equation,

$$Q_{\alpha\nu}(q_j) = Q^0_{\alpha\nu} + Q^{\Phi}_{\alpha\nu}(q_j) \tag{5}$$

is such that $Q_{\alpha\nu}(q_j)/2$ is an $\alpha\nu$ pseudofermion or hole overall phase shift. Indeed, if when moving around the lattice ring the $\alpha\nu$ pseudofermion or hole departs from the point $x = 0$ and arrives at $x = L/2$, one finds that $\lim_{x\rightarrow L/2}\bar{q}x = qx + Q_{\alpha\nu}(q)/2$ where $q$ refers to the initial ground state. From equations (2) and (5) it then follows that $\pi\Phi_{\alpha\nu,\alpha'\nu'}(q_j, q_{j'})$ is an elementary two-pseudofermion phase shift. (If instead one considers $x = 0$ and $x = L$, the overall phase shift and the two-pseudofermion phase shifts read $Q_{\alpha\nu}(q)$ and $2\pi\Phi_{\alpha\nu,\alpha'\nu'}(q_j, q_{j'})$, respectively [13]. However, the choice of definition is a matter of taste and the uniquely defined quantity is the above $S$ matrix.)

Several properties play an important role in the pseudofermion scattering theory. First, the elementary scattering processes associated with the phase factor (3) conserve the total energy and total momentum. Second, the elementary scattering processes are of forward-scattering type and thus conserve the individual in asymptote $\alpha\nu$ pseudofermion or hole momentum and energy. These processes also conserve the $\alpha\nu$ branch, usually called the *channel* in scattering language. Moreover, the scattering amplitude does not connect objects with different $\eta$-spin or spin. Last but not least, for each $\alpha\nu$ pseudofermion or hole of initial ground-state momentum $q_j$, the $S$ matrix associated with the ground-state–excited-energy-eigenstate transition is simply the phase factor given in equation (4). For each excited energy eigenstate (out asymptote) the number of $\alpha\nu$ pseudofermions plus the number of $\alpha\nu$ pseudofermion holes whose $S$ matrix is of the form (4) is given by $N_a + N^*_{s1} + \sum_{\alpha\nu\neq c0,s1}\theta(|\Delta N_{\alpha\nu}|)N^*_{\alpha\nu}$. Here $\theta(x) = 1$ for $x > 0$ and $\theta(x) = 0$ for $x = 0$.

Importantly, the form of the scattering part of the overall phase shift (5), equation (2), reveals that the value of such a phase shift functional is independent of the changes in the occupation numbers of the $\pm 1/2$ Yang holons and $\pm 1/2$ HL spinons. Thus, these objects are not scattering centres. Moreover, they are not scatterers, once their momentum values remain unchanged under the ground-state–excited-energy-eigenstate transitions. In turn, the pseudofermions and holes are scatterers and scattering centres. Since the $c0$ pseudofermion is a $\eta$-spinless and spinless object and for $\nu > 0$ the $\alpha\nu$ pseudofermions are $\eta$-spin ($\alpha = c$) and spin ($\alpha = s$) singlet $2\nu$-holon and $2\nu$-spinon composite objects, respectively, their $S$ matrix has dimension one: it is the phase factor (4). The factorization of the Bethe-ansatz (BA) bare $S$ matrix for the original spin-$1/2$ electrons is associated with the so called Yang–Baxter equation (YBE) [7]. On the other hand, the factorization of the $S$ matrix (4) in terms of the elementary $S$ matrices $S_{\alpha\nu,\alpha'\nu'}(q_j, q_{j'})$, equation (3), is commutative. Such a commutativity is stronger than the symmetry associated with the YBE and results from the elementary $S$ matrices $S_{\alpha\nu,\alpha'\nu'}(q_j, q_{j'})$ being simple phase factors, instead of matrices of dimension larger than one. This seems to be inconsistent with all PS energy eigenstates being described by occupancy configurations which, besides $c0$ pseudofermions, involve finite spin-$1/2$ spinons and $\eta$-spin-$1/2$ holons [10]. Indeed, the $S$ matrix of finite $\eta$-spin or spin objects has dimension larger than one. However, due to the correlations the quantum liquid self-organizes in such a way that the scatterers and scattering centres are the $c0$ pseudofermions, $\eta$-spin singlet $2\nu$-holon composite $c\nu$ pseudofermions, and spin singlet $2\nu$-spinon composite $s\nu$ pseudofermions.

Let us clarify how the $\alpha\nu$ pseudofermion $S$ matrix (4) controls the unusual spectral properties of the model. Consider an $\alpha\nu$ pseudofermion of canonical momentum $\bar{q}$ and an $\alpha'\nu'$ pseudofermion of canonical momentum $\bar{q}'$ such that the values $\bar{q}$ and $\bar{q}'$ correspond to a PS excited energy eigenstate and the initial ground state, respectively, and thus $\bar{q}' = q'$. Importantly, from the use of equation (4) it is found that the pseudofermion anticommutation relations introduced in [3] can be expressed solely in terms of the difference $[\bar{q} - \bar{q}']$ and the $S$ matrix of the $\alpha\nu$ pseudofermion associated with the excited state,

$$\{f^{\dagger}_{\bar{q},\alpha\nu}, f_{\bar{q}',\alpha'\nu'}\} = \delta_{\alpha\nu,\alpha'\nu'}\frac{1}{N^*_{\alpha\nu}}[S_{\alpha\nu}(q)]^{1/2}\mathrm{e}^{-\mathrm{i}(\bar{q}-\bar{q}')/2}\frac{\mathrm{Im}[S_{\alpha\nu}(q)]^{1/2}}{\sin([\bar{q} - \bar{q}']/2)}, \qquad (6)$$

and the anticommutators of two creation or annihilation operators vanish. This reveals that the $S$ matrix (4) fully controls the pseudofermion anticommutators. Since within the PDT these anticommutators determine the value of the matrix elements connecting energy eigenstates [4], it follows that the $S$ matrix (4) controls the spectral properties. If it had dimension larger than one, the pseudofermion algebra would be much more involved, for the pseudofermion anticommutators would also be matrices of dimension larger than one.

In [8] the excited states generated from the $n = 1$ and $m = 0$ ground state were described in terms of $\pm 1/2$ holon and $\pm 1/2$ spinon occupancy configurations. Following the analysis of [11, 12] for the related spin-1/2 isotropic Heisenberg chain, the holes of the BA length-one spin string spectrum (spin singlet two-spinon composite $s1$ pseudoparticle spectrum) were identified in [8] with the spinons. Inspired by such an interpretation, the studies of the latter reference identified the holons with the holes of the BA distribution of $k'$s [2, 10] spectrum ($c0$ pseudoparticle spectrum). This is behind the charge $\pm e$ found for the $\pm 1/2$ holons in [8], which is half of the value found in [10]. However, the $c0$ pseudoparticle and hole band occupancy configurations do not correspond to $\eta$-spin $SU(2)$ irreducible representations. Indeed, in [10] it is shown that for the whole Hilbert space all such representations exactly correspond to the BA charge string and $\mp 1/2$ Yang holon occupancy configurations. Following directly the analysis of [11, 12], the studies of [8] consider that the $\pm 1/2$ holons and $\pm 1/2$ spinons are the scatterers and scattering centres. This leads to two $4 \times 4$ $S$ matrices for holons and spinons, respectively, and a related $16 \times 16$ $S$ matrix for the full scattering problem. In spite of being mathematically elegant and obeying the YBE, these matrices are not suitable for the description of the spectral properties. Moreover, provided that within the $x = 0$ and $x = L$ boundary conditions one defines the overall phase shift as $Q_{\alpha\nu}(q)$, the phase shifts given in equations (5.19)–(5.21) of the first paper of [8], which appear in the entries of these matrices, are nothing but very particular cases of $\eta$-spinless and spinless $c0$ pseudofermion hole or spin-zero $s1$ pseudofermion hole overall phase shifts given in equation (5) [13]. Indeed, these phase shifts correspond to the $n = 1$ and $m = 0$ initial ground state and the specific excited states considered in [7, 8]. Let $q_1$ or $q'_1$ be the bare momenta of the scattered $c0$ or $s1$ pseudofermion hole, respectively, of the latter states. For the $\eta$-spin triplet, $\eta$-spin singlet, and $\eta$-spin and spin doublet excited states considered in these references, it is found that $\pi + Q_{c0}(q_1)$ equals the phase shift $\delta_{CT}$ and $\delta_{CS}$ given in equation (5.19) and $\delta_{\eta S}$ in equation (5.21) of the above paper, respectively. For the spin triplet, spin singlet, and spin and $\eta$-spin doublet excited states, $Q_{s1}(q'_1)$ equals the shift functions $\delta_{ST}$ and $\delta_{SS}$ given in equation (5.20) and $\delta_{S\eta}$ given in equation (5.21), respectively [13]. Thus, the BA phase shifts of [7, 8] are particular cases of the $c0$ and $s1$ pseudofermion hole overall phase shift functionals of equation (5) and are associated with a set of excited states which span a subspace smaller than the PS of the one- and two-electron excitations. According to the studies of [10], for all the transitions associated with these phase shifts the deviations in the $\eta$-spin and spin values are provided by the $\pm 1/2$ Yang holon and $\pm 1/2$ HL spinon occupancy changes, respectively, which do not contribute to the phase shift values. In turn, the holes created in the $c0$ and $s1$ bands by these transitions are both scatterers and scattering centres and it follows from the analysis of [10] that they do not correspond to single $\pm 1/2$ holons and $\pm 1/2$ spinons, respectively. Moreover, the phase shifts of [7, 8] were evaluated up to an overall constant term by the method of [14]. Equation (5) provides the full phase shift value and reveals that the above extra $\pi$ in $\delta_{CT}$, $\delta_{CS}$, and $\delta_{\eta S}$ is not physical, as discussed elsewhere [13]. The results reported here also apply to other models. For instance, for the isotropic Heisenberg chain it is found that the phase changes for the spin singlet and triplet excited states given in equation (11) of [11] equal the phase shifts for the same states of a scattered hole of the zero-spin two-spinon $s1$ pseudofermion spectrum. Thus, for the study of the spectral properties, these two excited states correspond to two $s1$ pseudofermion hole $S$

matrices, rather than to the single $4 \times 4$ $S$ matrix of equation (5.1) of [12]. This analysis can also be extended to the same model with an odd number of lattice sites.

While, through the anticommutators (6), the use of the $S$-matrix introduced here leads to a successful description of the spectral features observed for real materials [5], the $16 \times 16$ $S$ matrix of [8] is unsuitable for such a task. Indeed, independent $\pm 1/2$ holons and $\pm 1/2$ spinons that are not part of composite pseudofermions are neither scatterers nor scattering centres. Interestingly, these objects remain invariant under the electron–rotated-electron unitary transformation, whereas the pseudofermions and holes are not in general invariant under such a transformation.

The method for evaluation of the finite-energy spectral weight distributions of a 1D correlated metal introduced in [4] fully relies on the scattering theory introduced here. The exotic metallic quantum phase of matter found for quasi-1D compounds [5] by use of such a method is expected to emerge at finite energies in carbon nanotubes, ballistic wires, and systems of cold fermionic atoms in one-dimensional optical lattices with on-site atomic repulsion [9]. This confirms the general scientific interest of the scattering theory introduced here. While in this work it is applied specifically to the 1D Hubbard model, the theory is of general nature for many integrable quantum problems and therefore will have wide applicability.

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