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Andreas Osterloh, Luigi Amico, Ulrich Eckern

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Andreas Osterloh [a,*], Luigi Amico [b], Ulrich Eckern [a]

[a] *Institut für Physik,Universität Augsburg, D-86135 Augsburg, Germany*
[b] *Dipartimento di Metodologie Fisiche e Chimiche per l'Ingegneria, Facoltá di Ingegneria,*
Universitá di Catania & INFM, viale A. Doria 6, I-95129 Catania, Italy

Abstract

A class of integrable one-dimensional models presented by Shastry and Schulz is consequently extended to the whole class of one-dimensional Hubbard- or XXZ-type models with correlated gauge-like hopping. A complete characterization concerning solvability by coordinate Bethe ansatz of this class of models is found.

1. Introduction

Integrability has been considered to be one of the most striking properties of a model for some time. However, the interest was confined to an abstract level since integrable quantum systems typically live in one spatial dimension (but they can be mapped onto classical $(1 + 1)$-dimensional systems [1,2]). In the meantime, one-dimensional systems have become experimental reality (Quantum Hall bars [3,4], polymers [5], charge density wave systems [6]) and thus integrable models have gained immediate relevance for real physical problems. The Coordinate Bethe ansatz (CBA) [7–10] solvability is the first milestone in proving integrability. The (Quantum) Inverse Scattering Method together with the algebraic Bethe ansatz complete the CBA procedure to construct integrable models [1,11]. However, the interrelation between solvability by algebraic Bethe ansatz and CBA is still controversial. But solvability by algebraic Bethe ansatz is a strong hint for solvability by CBA within an appropriately chosen basis. In the case of the quantum

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* Corresponding author.
  E-mail address: andreas.osterloh@physik.uni-augsburg.de (A. Osterloh).

impurity problems, for instance, the standard CBA procedure with plane waves fails, in contrast to using a basis consisting of solitary waves [2,12]. The reason for this is that the bulk theory already describes fully interacting electrons and there is no (free) single particle description of the system. As a result the scattering with the impurity is "diffractive" in the plane-wave basis. Instead, it turns out to be factorizable if the many-electron wave function is written in terms of kinks and anti-kinks.

A breakthrough in the theory of integrable models was the solution of the Hubbard Model (HM) obtained by E.H. Lieb and F.Y. Wu [13]. The HM is a model including on-site Coulomb interaction for electrons moving in an atomic lattice. It is believed to capture important features of high-T_C superconductivity [14] and has a metal–insulator transition.

In a recent paper, H.J. Schulz and B.S. Shastry found a new class of solvable one-dimensional Hubbard- and XXZ-type models [15]. The modification of the original HM and XXZ model consisted in a configuration dependent unitary factor in the hopping term. This can be interpreted as an interaction of the charged particles with a gauge-field, generated by the density of particles. The structure of the unitary factor was $\exp[i\widehat{N}]$, where $\widehat{N}$ is a mono-linear functional of particle-number operators; we term such models "single particle correlated hopping (1-CH)" models.

The idea behind Schulz' and Shastry's approach is finding a basis (through a unitary transformation of the original Fock basis) in which the model takes the form of the original Hubbard or XXZ model up to boundary twists which do not affect their solvability [16]. We point out that this is equivalent to equipping the plane waves entering the CBA with phase factors canceling exactly the configuration dependent gauge fields in the hopping term. In the present paper we will generalize such an idea to consider hopping in which $\widehat{N}$ is a multilinear functional of particle-number operators. We shall call the resulting models n-CH models. We will answer the question which n-CH-Hubbard/XXZ models can be mapped unitarily onto a corresponding uncorrelated but twisted model. This finally proves solvability of the model. Conversely, a non-removable correlated hopping destroys solvability by CBA, since the S matrix becomes configuration dependent (see Appendix A).

The paper is laid out as follows. In Section 2, we will study the most general form of 1-CH HMs, hence including Shastry–Schulz models. Most of the features of the general problem already occur here. Section 3 accounts for conserved quantum numbers other than the spin orientation of electrons. Multi-chain models where the chains interact with each other exclusively gauge-like, will be considered. The central results obtained in Sections 2 and 3 will be used to discuss higher correlated hopping in Section 4. The 2-CH will be treated in detail, enlightening the approach to general n-CH.

A special class of unitary transformations was used to remove the gauge-like correlation terms from the hopping. In Appendix C the effect of the complementary class of unitary transformations will be elaborated, always restricting on automorphic mappings on the class of twisted n-CH models of Hubbard- or XXZ-kind. Two propositions needed in this section will be proven in the appendix. Finally, conclusions will be drawn in Section 5.

2. Single-particle correlated hopping

In this section we discuss a simple generalization of Schulz–Shastry models. Such models have the following Hubbard-type Hamiltonian

$$H = -t \sum_{j,\sigma} c^\dagger_{j+1,\sigma} c_{j,\sigma} \exp\left(i\gamma_j(\sigma)\right)$$

$$\times \exp\ i \sum_l \left(\alpha_{j,l}(\sigma)n_{l,-\sigma} + A_{j,l}(\sigma)n_{l,\sigma}\right) \quad + \text{h.c.}$$

$$+ V \sum_i n_{i,\uparrow} n_{i,\downarrow}, \tag{1}$$

where $\{c_{j,\sigma}, c^\dagger_{l,\sigma'}\} = \delta_{\sigma,\sigma'}\delta_{j,l}$, $\{c_{j,\sigma}, c_{l,\sigma'}\} = 0$, and $n_{l,\sigma} := c^\dagger_{l,\sigma}c_{l,\sigma}$. The parameters t, V are the hopping amplitude and the Coulomb repulsion, respectively. The class of models (1) is a generalization of Schulz–Shastry models, since (a) the parameter A occurs, which means correlation between particles with the same spin orientation, and (b) the spin and coordinate dependence of A, α, γ is unrestricted here. [1]

We point out that $A_{j,j+1}$ can be set to an arbitrary value for all j, without affecting the physics of the model (since $n_{l,\sigma} \in \{0, 1\} \Rightarrow c^\dagger_{j+1,\sigma}n_{j+1,\sigma} \equiv 0$). We name parameters like $A_{j,j+1}$ "irrelevant". A similar argument holds for the parameter $A_{j,j}$: contributions from $n_{j,\sigma}$ arise only if $n_{j,\sigma} = 1$ because of $c_{j,\sigma}n_{j,\sigma} \equiv c_{j,\sigma}$. Hence, this term can be included in the parameter $\gamma_j(\sigma)$. Parameters like $A_{j,j}$ will be called "subrelevant" throughout this paper. Irrelevant as well as subrelevant parameters appear as soon as phase-correlations among particles having the same spin orientation as the hopping particle are involved.

It is worthwhile noting that Hamiltonian (1) is not diagonalizable by *direct* CBA since the scattering matrix is configuration dependent (see Appendix A). This destroys the factorizability of a many-particle S matrix into two-particle S matrices. Thus, we first remove the phases in the hopping term of (1) by a unitary transformation and then, we can diagonalize the transformed Hamiltonian by CBA.

The ansatz for the unitary transformation is achieved through the operator

$$U := \exp\ i\left(\xi^{\mu,\nu}_{l,m} n_{l,\mu}n_{m,\nu} + \zeta_{l,\mu}n_{l,\mu}\right) =: \exp(iS), \tag{2}$$

(we use the sum convention) where $\xi_{i,j}$, $\zeta_{l,m} \in \mathbb{R}$ are unknown variables which have to be fixed for cancelling the unitary prefactor in the hopping term of (1). Since an antisymmetric part in the parameter $\xi_{i,j}$ vanishes after summation, it can be defined fully symmetric: $\xi^{\mu,\nu}_{l,m} = \xi^{\nu,\mu}_{m,l}$. We can further choose $\xi^{\mu,\mu}_{m,m} = 0$ (a non-zero $\xi^{\mu,\mu}_{m,m}$ can be included in the parameter $\zeta_{l,m}$).

We locally transform the Hamiltonian by $U: c_{j,\sigma} \xrightarrow{U} U c_{j,\sigma} U^{-1}$. Number operators remain unchanged, but the hopping term is altered

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[1] For spin 1/2 every function of $f(\sigma)$ is linear in σ: $f(\sigma) =: f_0 + \sigma f_1$, where f_0 and f_1 are constant. In the Ref. [15] only $\alpha(\sigma)$ exists, which there was chosen to be a periodic translational invariant function of the site indices. Additionally, $\alpha(\sigma) = \sigma\alpha_1$ was taken.

$$c^\dagger_{j+1,\sigma} c_{j,\sigma} \xrightarrow{U} c^\dagger_{j+1,\sigma} c_{j,\sigma} \exp 2\mathrm{i}\big(\xi^{\sigma,\mu}_{j+1,m} - \xi^{\sigma,\mu}_{j,m}\ n_{m,\mu}$$
$$\times \exp \mathrm{i}\big(\zeta_{j+1,\sigma} - \zeta_{j,\sigma} - 2\xi^{\sigma,\sigma}_{j,j+1}\big) \quad .$$

The unitary factors in the hopping term of (1) are removed if

$$2\big(\xi^{\sigma,-\sigma}_{j,m} - \xi^{\sigma,-\sigma}_{j+1,m}\big) \overset{!}{=} \alpha_{j,m}(\sigma), \tag{3}$$

$$\big(\zeta_{j,\sigma} - \zeta_{j+1,\sigma} + 2\xi^{\sigma,\sigma}_{j,j+1} \overset{!}{=} \gamma_j(\sigma), \tag{4}$$

and

$$2\big(\xi^{\sigma,\sigma}_{j,m} - \xi^{\sigma,\sigma}_{j+1,m} \overset{!}{=} A_{j,m}(\sigma), \quad m \in \{1,\dots,L\} \setminus \{j, j+1\}. \tag{5}$$

For periodic boundary conditions (PBC), Eqs. (3)–(5) for $j = L$ represent the jump across the boundary. Admitting boundary phases in company with the boundary's crossing, Eqs. (3)–(5) are modified as

$$2\big(\xi^{\sigma,-\sigma}_{L,m} - \xi^{\sigma,-\sigma}_{1,m}\big) \overset{!}{=} \alpha_{L,m}(\sigma) - \phi^{(1)}_{\uparrow\downarrow}(\sigma), \tag{6}$$

$$\big(\zeta_{L,\sigma} - \zeta_{1,\sigma} + 2\xi^{\sigma,\sigma}_{L,1} \overset{!}{=} \gamma_L(\sigma) - \phi(\sigma), \tag{7}$$

and

$$2\big(\xi^{\sigma,\sigma}_{L,m} - \xi^{\sigma,\sigma}_{1,m} \overset{!}{=} A_{L,m}(\sigma) - \phi^{(1)}_{\uparrow\uparrow}(\sigma), \quad m \in \{2,\dots,L-1\}. \tag{8}$$

In fact, the relations (3)–(5) and (6)–(8) constitute a system of recursive relations for $\xi^{\sigma,\sigma'}_{j,m}$ and $\zeta_{j,\sigma}$.

We will now discuss the exclusions in Eq. (5). The corresponding part of the transformed hopping term for $m = j$ is (since $\xi^{\sigma,\sigma}_{j,j} = 0$) $c^\dagger_{j+1,\sigma} c_{j,\sigma} \exp[\mathrm{i}(2\xi^{\sigma,\sigma}_{j+1,j} + A_{j,j}(\sigma))n_{j,\sigma}]$. This term is non-zero only if $n_{j,\sigma} = 1$. Hence, this "correlation" factor is equivalent to $c^\dagger_{j+1,\sigma} c_{j,\sigma} \exp[\mathrm{i}(2\xi^{\sigma,\sigma}_{j+1,j} + A_{j,j}(\sigma))]$. For $m = j + 1$ it is $c^\dagger_{j+1,\sigma} c_{j,\sigma} \exp[-\mathrm{i}(2\xi^{\sigma,\sigma}_{j,j+1} - A_{j,j+1}(\sigma))n_{j+1,\sigma}]$. This term is non-zero only if $n_{j+1,\sigma} = 0$. Hence, this "correlation" factor is equivalent to $c^\dagger_{j+1,\sigma} c_{j,\sigma}$ irrespective of what value $A_{j,j+1}(\sigma) - 2\xi^{\sigma,\sigma}_{j,j+1}$ may take. As a consequence, there is no condition for $m = j + 1$ in Eq. (5), and $A_{j,j}(\sigma) + 2\xi^{\sigma,\sigma}_{j,j+1}$ enters as a modification of Eq. (4) for γ_j (see Appendix B). The system of Eqs. (3)–(4) cannot be solved for arbitrary α and A (the number of parameters on the right-hand side is larger than on the left-hand side). Together with the symmetry of $\xi_{i,j}$, Eqs. (3) and (5) define the effect of an increase in both site indices of $\xi_{i,j}$; namely an increase of ξ by the related α, respectively A. Starting from an initial parameter, say $\xi_{1,1} := 0$, every $\xi_{i,j}$ is then defined by passing from $(1, 1)$ to (i, j) and summing up the contributions from the recursive relation. $\xi_{i,j}$ is well defined if this procedure is path independent. This is equivalent to demanding that contributions from closed loops in the (i, j) plane vanish. To verify this, it is sufficient facing the smallest possible loops: $(j, m) \to (j + 1, m) \to (j + 1, m + 1) \to (j, m + 1) \to (j, m)$ (which we will henceforth call "elementary"). Applying Eq. (3), respectively Eq. (5), we obtain

$$\alpha_{j,m+1}(\sigma) - \alpha_{j,m}(\sigma) = \alpha_{m,j+1}(-\sigma) - \alpha_{m,j}(-\sigma), \tag{9}$$

and

$$A_{j,m+1}(\sigma) - A_{j,m}(\sigma) = A_{m,j+1}(\sigma) - A_{m,j}(\sigma) \tag{10}$$

for $m \neq j, j \pm 1$. We call the conditions (9), (10) "closedness conditions". The recursive relation and the closedness condition can be written in a more compact and clear form in terms of the discrete gradient, defined by $\partial_x f(x) := f(x+1) - f(x)$. The recursive relations (3) and (5) then read

$$-2\partial_x \xi^{\sigma,-\sigma}(x,y) \equiv -2\partial_x \xi^{-\sigma,\sigma}(y,x) = \alpha(x,y;\sigma), \tag{11}$$

$$-2\partial_x \xi^{\sigma,\sigma}(x,y) \equiv -2\partial_x \xi^{\sigma,\sigma}(y,x) = A(x,y;\sigma) \tag{12}$$

and the closedness conditions take the form

$$\partial_y \alpha(x,y;\sigma) = \partial_x \alpha(y,x;\sigma), \tag{13}$$

$$\partial_y A(x,y;\sigma) = \partial_x A(y,x;\sigma), \quad x \neq y. \tag{14}$$

With these conditions being fulfilled,[2] the correlations from the hopping term can be removed and the rotated model is finally known to be solvable by CBA.

For open boundary conditions the correlated hopping can be "gauged away" completely, yielding the HM without any boundary phases.

Instead, PBC lead to the HM with twisted boundary conditions. Periodicity implies that the parameters $\xi_{i,j}$, α, A and γ are periodic in their site-indices with period L. The boundary phase is determined by hopping from site L to site $L + 1 \hat{=} 1$; such a phase enters as written in Eqs. (6)–(8) for the relations $\xi_{1,m} \leftrightarrow \xi_{L,m}$ and $\zeta_{1,m} \leftrightarrow \zeta_{L,m}$ and then for $A_{1,m} \leftrightarrow A_{L,m}$, $\alpha_{1,m} \leftrightarrow \alpha_{L,m}$. Eqs. (3)–(8) lead to

$$2\left(\xi_{1,m}^{\sigma,-\sigma} - \xi_{L,m}^{\sigma,-\sigma}\right) = \sum_{j=1}^{L-1} \alpha_{j,m}(\sigma) \stackrel{!}{=} -\alpha_{L,m}(\sigma) + \phi_{\uparrow\downarrow}^{(1)}(\sigma), \tag{15}$$

$$2\left(\xi_{1,m}^{\sigma,\sigma} - \xi_{L,m}^{\sigma,\sigma}\right) = \sum_{\substack{j=1 \\ j \neq m, m-1}}^{L-1} A_{j,m}(\sigma) + 2\left(\xi_{m-1,m}^{\sigma,\sigma} - \xi_{m,m+1}^{\sigma,\sigma}\right)$$

$$\stackrel{!}{=} -A_{L,m}(\sigma) + \phi_{\uparrow\uparrow}^{(1)}(\sigma), \tag{16}$$

$$\zeta_{1,\sigma} - \zeta_{L,\sigma} = \sum_{j=1}^{L-1}\left(\gamma_j(\sigma) + A_{j,j}\right) \stackrel{!}{=} -\gamma_L(\sigma) - A_{L,L} + \phi(\sigma), \tag{17}$$

where ϕ denotes the boundary phases. They can be determined (without solving for the ξ's explicitly) from Eqs. (15)–(17) as

$$\phi_{\uparrow\downarrow}^{(1)}(\sigma) = \sum_{j=1}^{L} \alpha_{j,m}(\sigma), \tag{18}$$

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[2] In fact the phases have to be removed modulo 2π only, which therefore also holds for the closedness conditions. However, having a parameter which scales the strength of the correlation (i.e., $A_{j,m,\dots}^{\sigma,\mu,\dots} = \varphi \tilde{A}_{j,m,\dots}^{\sigma,\mu,\dots}$), the equations are not to be taken modulo 2π as far as solvability for arbitrary values of φ is concerned. Also for this reason mod2π is omitted throughout the paper.

$$\phi_{\uparrow\uparrow}^{(1)}(\sigma) = \sum_{\substack{j=1 \\ j \neq m-1,m}}^{L} A_{j,m}(\sigma) + A_{m,m-1}(\sigma) + A_{m-1,m+1}(\sigma), \tag{19}$$

$$\phi(\sigma) = \sum_{j=1}^{L} \left(\gamma_j(\sigma) + A_{j,j}(\sigma) \right). \tag{20}$$

Eqs. (9) and (10) also ensure that the phases in Eqs. (18) and (19) are m-independent.[3] Summarizing, *iff* Eqs. (9) and (10) are fulfilled, the Hamiltonian (1) can be mapped by U (Eq. (2)) onto the usual HM with modified boundary conditions. The boundary twists are given by

$$\Phi_\sigma := \phi(\sigma) + \phi_{\uparrow\downarrow}^{(1)}(\sigma)N_{-\sigma} + \phi_{\uparrow\uparrow}^{(1)}(\sigma)(N_\sigma - 1). \tag{21}$$

We emphasize that here, the factor $(N_\sigma - 1)$ appears instead of N_σ. The reason is that the recursive relation (5) does not exist for $m = j, j + 1$. But since one particle with spin σ
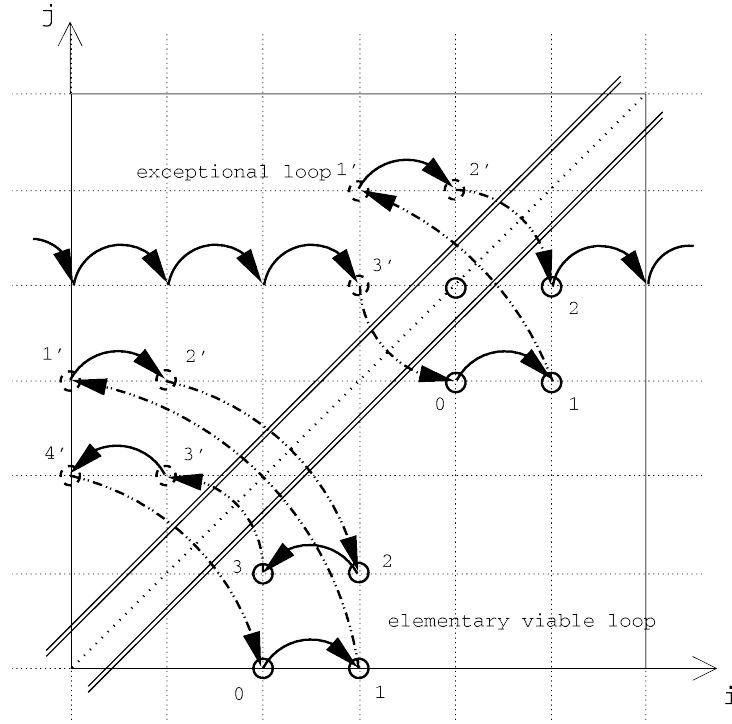

Fig. 1. Elementary viable (leading to (10)) and not elementarily viable (called "exceptional") loops, are drawn in the space of indices (i, j) of $\xi_{i,j}^{\sigma,\sigma}$ (the crossings of the dotted lines are the possible index points). The exceptional loop determines the boundary phase for the parameter A. Full arrows mean an application of the recursive relation (5), which can transport in horizontal direction only. The other arrows visualize the application of the symmetry $\xi_{i,j} = \xi_{j,i}$. The double lines are reminders of the missing connection between $\xi_{j-1,j}^{\sigma,\sigma}$ and $\xi_{j,j}^{\sigma,\sigma}$. Hence, it must not be crossed by the full arrows.

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[3] The phases (18) and (19) can also be obtained from calculating the contribution of the exceptional loop in Fig. 1 (respecting the formerly unknown boundary phases). Setting the contribution of this loop to zero determines the phase. In case of (18), no forbidden crossings exist, as mentioned before.

has to be on site j and none on site $j + 1$ (or vice versa: see the corresponding hopping term in (1)), one particle less accounts for the phase.

2.1. Translational invariant models

In this section we assume a translational invariant model, and hence translational invariance of the parameters α and A: $\alpha_{j,l}(\sigma) = \alpha_{j-l}(\sigma)$, $A_{j,l}(\sigma) = A_{j-l}(\sigma)$.

Restricting ourselves to translational invariant unitary transformations[4] ($\xi_{j,k} = \xi_{j-k}$), the former elementary loops become multiple loops (see Fig. 2). Then, the elementary loops are $(j, m) \to (j + 1, m) \to (j + 1, m + 1)$ and the closedness condition only consists of the following terms from Eqs. (9) and (10) $\alpha_j(\sigma) = -\alpha_{-(j+1)}(-\sigma)$ for all j, $A_j(\sigma) = -A_{-(j+1)}(\sigma)$ for all $j \neq 0$. Also here, for the parameter A not all elementary loops are viable. But the only exceptional loop emerges from the case corresponding to $m = j$ in Eq. (10) (that is a square on the diagonal — the fat dotted line in Fig. 1). But as already mentioned, the (excluded) condition for $m = j$ in Eq. (10) is trivially fulfilled. This is confirmed by calculating the effect of the jump from 0 to 2 in the exceptional loop in Fig. 1, which here constitutes an elementary loop (comparing with Fig. 2 it turns out that the points 0 and 2 are identified since translational invariant parameters are assumed). As a consequence, the feature of additional phases imported by subrelevant parameters and hence non-viable loops are absent here.

But we want to stress that even here Eqs. (9), (10) are necessary and sufficient conditions for solvability — for periodic as well as for open chains. This is because a translational
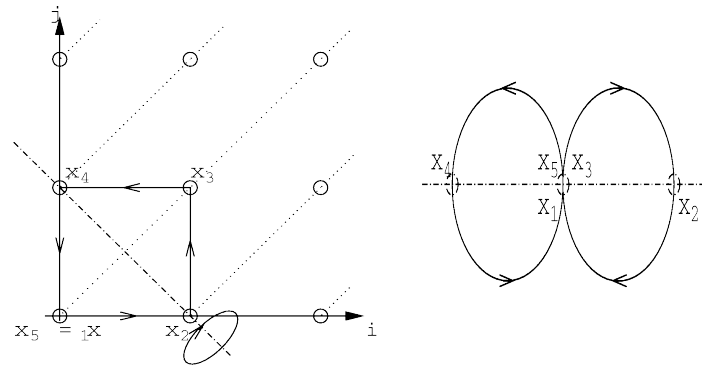

Fig. 2. On the left, an elementary loop in two-coordinate space is drawn. The circles are the coordinate sites, say (i, j), corresponding to a parameter $\xi_{i,j}$. If the parameters in the transformation are assumed depending on the difference of the coordinates only, the dotted lines connect identified sites in index space, corresponding to identical parameter values. One can imagine the resulting reduced lattice by furling the coordinate space along the dash-dotted line to a cylinder or by pushing the identified sites on each other, which is visualized on the right. In this case, the former elementary loop turns into a double loop. Each of these two loops is an elementary loop.

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[4] In fact, the unitary transformation need not be translational invariant even for a translational invariant model. Such an ansatz only means looking for a solution in a subset of unitary transformations. Hence, Eqs. (9), (10) are still necessary but no more sufficient for the closedness of the recursive relation for the translational invariant ansatz, but they are still for CBA solvability.

invariant model need not necessarily be gauged away by a unitary transformation with translational invariant parameters.

Now, we can connect to Ref. [15]. We obtain the boundary phases in Ref. [15] through the identifications $\alpha_{j,m} \to \alpha_{j-m}$ and $\alpha_j(\sigma) := -\sigma\alpha_j$. In addition, $A_{j,m}(\sigma) = \gamma_j(\sigma) \equiv 0$ and $\beta_{i,j} = \sigma/2 \cdot \xi_{i,j}^{\sigma,-\sigma}$, giving an antisymmetric $\beta_{i,j}$. However, in order to guarantee closedness and hence solvability of the recursive relations,

$$\alpha_{j-m} - \alpha_{j-m-1} = -(\alpha_{m-j} - \alpha_{m-j-1})$$

has to hold.

A special type of such models is studied in Ref. [17] with the only non-zero values $\alpha_0 = \alpha_{-1} = \eta$, where η is a real parameter. The closedness conditions are all fulfilled and therefore the correlation factors in the hopping can be gauged away giving exactly the phases found in [17]. However, we could not reproduce the results following the path suggested in [17] (see the general discussion in Appendix A).

3. Multi-chain models

Multi-chain models can be treated analogously. The chain-variable plays the role of the spin-variable now. The only difference is that in general the chain variable ranges in a set different from $\{-1/2, +1/2\}$. Since the method we employ to diagonalize the Hamiltonian stays the same, we only state the results. For multi-chain models we assume *intra-chain hopping only*.

At first, we deal with spin-less fermions and let the hopping-term of (1) take the form

$$a_{c,j+1}^{\dagger} a_{c,j} \exp\left(i\gamma_j(c) \ \exp \ iA_{j,l}^{c,d} n_{d,l} \ + \text{h.c.},\right. \tag{22}$$

where c and d are chain indices, which run in $\{1, \ldots, C\}$ with C being the number of chains.[5] The unitary transformation will be

$$U := \exp \ i\left(\xi_{l,m}^{\mu,\nu} n_{\mu,l} n_{\nu,m} + \zeta_{\mu,l} n_{\mu,l}\right., \tag{23}$$

where μ, ν are now site indices (instead of spin indices of Section 2), running in $\{1, \ldots, C\}$ (instead of $\{-1/2, 1/2\}$). In this case, the recursive relations are

$$2\left(\xi_{j,m}^{c,d} - \xi_{j+1,m}^{c,d} \ \overset{!}{=} A_{j,m}^{c,d}, \quad c \neq d,\right. \tag{24}$$

$$2\left(\xi_{j,m}^{c,c} - \xi_{j+1,m}^{c,c} \ \overset{!}{=} A_{j,m}^{c,c}, \quad m \neq j, j+1,\right. \tag{25}$$

$$\left(\zeta_{c,j} - \zeta_{c,j+1} + 2\xi_{j,j+1}^{c,c} \ \overset{!}{=} \gamma_{c,j}.\right. \tag{26}$$

The closedness conditions read

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[5] The chain index can also be interpreted as a color index, corresponding to some other inner degrees of freedom, characteristic for the particles. But all the models discussed here have in common that this index labels a good quantum number, corresponding to a conserved quantity. For models including color, color conservation is assumed.

$$A_{j,m+1}^{c,d} - A_{j,m}^{c,d} = A_{m,j+1}^{d,c} - A_{m,j}^{d,c}, \quad (c \neq d) \vee m \neq j \pm 1, \tag{27}$$

$$A_j^{c,d} = -A_{-(j+1)}^{d,c}, \quad c \neq d \vee j \neq 0, -1 \tag{28}$$

for all c, d, j, m respecting the noted exceptions. Eq. (28) applies to the translational invariant ansatz. The boundary phases finally become

$$\Phi_c = \phi_c + \sum_{d=1}^{C} \phi_c^{(1)}(d)(N_d - \delta_{c,d}), \tag{29}$$

where

$$\phi_c^{(1)}(d) = \sum_{j=1}^{L} A_{j,m}^{c,d}, \quad c \neq d, \tag{30}$$

$$\phi_c^{(1)}(c) = \sum_{\substack{j=1 \\ j \neq m-1,m}}^{L} A_{j,m}^{c,c} + A_{m,m-1}^{c,c} + A_{m-1,m+1}^{c,c}, \tag{31}$$

$$\phi_c = \sum_{j=1}^{L} \left(\gamma_{c,j} + A_{j,j}^{c,c} \right). \tag{32}$$

To compare this with Ref. [18], one has to replace $\xi_{l,m}^{\mu,\nu}$ with $\xi_{\mu,\nu} B_{\mu,\nu}(l-m)/2$ and additionally $A_{j,m}^{c,d}$ with $-\xi_{c,d} A_{c,d}(j-m)$. There, $\xi_{\mu,\nu}$ was antisymmetric and hence, $B_{\mu,\nu}(l-m)$ has to be antisymmetric, too: $B_{\mu,\nu}(m) = -B_{\nu,\mu}(-m)$. The solvability conditions (28) then transport into

$$\xi_{c,d} A_{c,d}(j-m) = -\xi_{d,c} A_{d,c}(m-j-1)$$
$$\iff \quad A_{c,d}(j-m) = A_{d,c}(m-j-1)$$

for all m, j, c, d. This is equivalent to $A_{c,d}(-m) = A_{d,c}(m-1)$ for all m, c, d as obtained in Ref. [18]. This condition is sufficient for CBA solvability but not necessary. Necessary and sufficient is $A_{c,d}(-m) - A_{d,c}(-m-1) - A_{c,d}(m-1) + A_{d,c}(m) = 0$ for all m.

If spin has to be included, nothing changes but the number of indices. The hopping term becomes

$$a_{c,j+1;\sigma}^{\dagger} a_{c,j;\sigma} \exp\left(i\gamma_j(c) \right) \exp i A_{j,l}^{c,d}(\sigma, \rho) n_{d,l;\rho} + \text{h.c.}, \tag{33}$$

where c, d are the chain indices again and σ, ρ are spin indices. The unitary transformation takes the form

$$U := \exp i \left(\xi_{l,m}^{\mu,\nu}(\rho, \tau) n_{\mu,l;\rho} n_{\nu,m;\tau} + \zeta_{\mu,l;\rho} n_{\mu,l;\rho} \right), \tag{34}$$

where μ, ν are the chain indices and ρ, τ are spin indices. The recursion relations read

$$2\left(\xi_{j,m}^{c,d}(\sigma, \rho) - \xi_{j+1,m}^{c,d}(\sigma, \rho) \right) \overset{!}{=} A_{j,m}^{c,d}(\sigma, \rho),$$
$$c \neq d \vee \sigma \neq \rho \vee m \neq j, j+1, \tag{35}$$

$$\left(\zeta_{c,j}(\sigma) - \zeta_{c,j+1}(\sigma) + 2\xi_{j,j+1}^{c,c}(\sigma, \sigma) \right) \overset{!}{=} \gamma_{c,j}(\sigma), \tag{36}$$

and the closedness conditions are

$$A_{j,m+1}^{c,d}(\sigma, \rho) - A_{j,m}^{c,d}(\sigma, \rho) = A_{m,j+1}^{d,c}(\rho, \sigma) - A_{m,j}^{d,c}(\rho, \sigma),$$
$$c \neq d \vee \sigma \neq \rho \vee m \neq j \pm 1 \tag{37}$$

for all c, d, j, m, σ, ρ respecting the exceptions. [6] The boundary phases become

$$\Phi_{c,\sigma} = \phi_{c,\sigma} + \sum_{d=1}^{C} \sum_{\mu \in \{\uparrow, \downarrow\}} \phi_{c,\sigma}^{(1)}(d, \rho)(N_{d,\rho} - \delta_{c,d}\delta_{\rho,\sigma}), \tag{38}$$

where

$$\phi_{c,\sigma}^{(1)}(d, \rho) = \sum_{j=1}^{L} A_{j,m}^{c,d}(\sigma, \rho), \quad c \neq d \vee \sigma \neq \rho, \tag{39}$$

$$\phi_{c,\sigma}^{(1)}(c, \sigma) = \sum_{\substack{j=1 \\ j \neq m-1, m}}^{L} A_{j,m}^{c,c}(\sigma, \sigma) + A_{m,m-1}^{c,c}(\sigma, \sigma) + A_{m-1,m+1}^{c,c}(\sigma, \sigma), \tag{40}$$

$$\phi_{c,\sigma} = \sum_{j=1}^{L} \left(\gamma_{c,j}(\sigma) + A_{j,j}^{c,c}(\sigma, \sigma) \right). \tag{41}$$

The overlap of Ref. [15] with the work presented in the Refs. [19,20] was discussed by the authors and was argued to not exist [18,21]. Now it is shown that the correlation in Refs. [19,20] cannot be gauged away, since the correlation parameters violate Eq. (37). However, the Hamiltonian having the slightly but essentially different phases

$$\exp\left[-i\pi\varphi_\sigma \left(n_{l+1,m,\sigma} - n_{l-1,m,\sigma} + n_{l+1,m+1,\sigma} - n_{l-1,m+1,\sigma} \right) + \frac{2\pi\gamma_\sigma}{N_a} \right] \tag{42}$$

instead of

$$\exp\left[-i\pi\varphi_\sigma \left(n_{l+1,m,\sigma} - n_{l-1,m,\sigma} \right) + \frac{2\pi\gamma_\sigma}{N_a} \right] \tag{43}$$

yields the BE found in Ref. [20].

The models studied in Ref. [22] are equivalent to multi-chain models of spin-less fermions. In the first model, the only non-zero model parameters are $A_{j,j}^{m,m+1} = -A_{j,j+1}^{m+1,m} = -4\Theta_{m,m+1}$ and $\gamma_j(m) = 2(\Theta_{m+1,m} - \Theta_{m,m-1})$, where we used the notation in [22]: j and m are the site and chain index, respectively. The second model is represented by the parameters $A_{j,j+1}^{m+1,m} = -A_{j,j}^{m,m+1} = \Theta_{m,m+1} + \alpha_{m,m+1}$ and $A_{j,j}^{m+1,m} = -A_{j,j+1}^{m,m+1} = \Theta_{m,m+1} - \alpha_{m,m+1}$. The closedness conditions are fulfilled *iff* $\Theta_{m,m+1} = \Theta_{m+1,m}$ and $\alpha_{m,m+1} = \alpha_{m+1,m}$.

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[6] In fact, spin and chain variables could be combined into a multi-index. Then the spin had the effect of doubling the number of chains.

4. Two-particle and higher correlated hopping

The procedure developed in the previous section can be extended to consider higher (than one-particle) correlated hopping. First, we face explicitly 2-particle correlated hopping (2-CH). Then we will sketch how to deal with the general case of n-CH.

2-CH corresponds to the occurrence of a term like $\bar{\alpha}_{l,m}^{\lambda,\mu}(j,\sigma)n_{l,\lambda}n_{m,\mu}$ in the exponential factor of the hopping term of (1). The 2-CH Hubbard-type Hamiltonian is

$$H = -t \sum_{j,\sigma} \left\{ c_{j+1,\sigma}^{\dagger} c_{j,\sigma} \exp\!\left(\mathrm{i}\gamma_j(\sigma) \ \exp \ \mathrm{i}\bar{\alpha}_{l,m}^{\lambda,\mu}(j,\sigma)n_{l,\lambda}n_{m,\mu} \right. \right.$$

$$\left. \left. \times \exp \ \mathrm{i}\alpha_m^{\mu}(j,\sigma)n_{m,\mu} \ + \text{h.c.} \right\} + V \sum_i n_{i,\uparrow}n_{i,\downarrow}. \tag{44}$$

Without loss of generality the parameters $\bar{\alpha}_{l,m}^{\lambda,\mu}(j,\sigma)$ can be chosen symmetric in the index pairs (l,λ) and (m,μ) and vanishing if these index pairs coincide. [7]

The parameters $\bar{\alpha}_{j+1,m}^{\sigma,\mu}(j,\sigma)$ and $\alpha_{j+1}^{\sigma}(j,\sigma)$ are irrelevant for all j,m,σ,μ; the effect of the subrelevant parameters on the lower correlated ones will be discussed later on in the present section.

We first remove the phases in the hopping term of (44) by a unitary transformation. Then, we diagonalize the transformed Hamiltonian by CBA in computing the boundary phases. The 2-CH demands an exponent $\bar{\xi}_{l,m,r}^{\lambda,\mu,\rho}n_{l,\lambda}n_{m,\mu}n_{n,\rho}$ in the unitary transformation U:

$$U := \exp \ \mathrm{i}\!\left(\bar{\xi}_{l,m,r}^{\lambda,\mu,\rho}n_{l,\lambda}n_{m,\mu}n_{r,\rho} + \xi_{l,m}^{\lambda,\mu}n_{l,\lambda}n_{m,\mu} + \zeta_{m,\mu}n_{m,\mu}\right)\Big]. \tag{45}$$

Both ξ and $\bar{\xi}$ are totally symmetric and vanish if any two pairs of parameters coincide.

The hopping term is transformed into

$$c_{j+1,\sigma}^{\dagger}c_{j,\sigma} \xrightarrow{\ U\ } c_{j+1,\sigma}^{\dagger}c_{j,\sigma} \exp\Big[3\mathrm{i}\big(\bar{\xi}_{j+1,l,m}^{\sigma,\lambda,\mu} - \bar{\xi}_{j,l,m}^{\sigma,\lambda,\mu}\big)n_{l,\lambda}n_{m,\mu}$$

$$+ 2\mathrm{i}\big(\xi_{j+1,m}^{\sigma,\mu} - \xi_{j,m}^{\sigma,\mu} - 3\bar{\xi}_{j,j+1,m}^{\sigma,\sigma,\mu}\big)n_{m,\mu}$$

$$+ \mathrm{i}\big(\zeta_{j+1,\sigma} - \zeta_{j,\sigma} - 2\xi_{j,j+1}^{\sigma,\sigma}\big) \Big],$$

whereas the Coulomb interaction term remains unchanged. This leads to the recursive relations (compare with (3)–(5))

$$3\big(\bar{\xi}_{j,l,m}^{\sigma,\lambda,\mu} - \bar{\xi}_{j+1,l,m}^{\sigma,\lambda,\mu}\big) \overset{!}{=} \bar{\alpha}_{l,m}^{\lambda,\mu}(j,\sigma),$$
$$(m \neq l \vee \mu \neq \lambda) \text{ and } (l,m \neq j, j+1 \vee \lambda, \mu \neq \sigma), \tag{46}$$

$$2\big(\xi_{j,m}^{\sigma,\mu} - \xi_{j+1,m}^{\sigma,\mu} + 3\bar{\xi}_{j,j+1,m}^{\sigma,\sigma,\mu}\big) \overset{!}{=} \alpha_m^{\mu}(j,\sigma), \quad m \neq j, j+1 \vee \mu \neq \sigma \tag{47}$$

$$\big(\zeta_{j,\sigma} - \zeta_{j+1,\sigma} + 2\xi_{j,j+1}^{\sigma,\sigma} \overset{!}{=} \gamma_j(\sigma), \tag{48}$$

for the parameters in U.

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[7] We point out that from now on we group the indices into blocks. Namely all indices of a corresponding number operator belong to one such block, containing a site- and a spin/color (multi-) index. An index exchange always means an exchange of a whole index block.

We point out that, in the present case, two kinds of elementary loops exist because of the variety of indices in $\bar{\alpha}_{l,m}^{\lambda,\mu}(j,\sigma)$. Namely: $(j;l,m) \to (j+1;l,m) \to (j+1;l+1,m) \to (j;l+1,m) \to (j;l,m)$ and $(j;l,m) \to (j+1;l,m) \to (j+1;l,m+1) \to (j;l,m+1) \to (j;l,m)$. However, due to the symmetry of the $\bar{\alpha}$ both loops give the same closedness condition for $\bar{\alpha}$, which is

$$\bar{\alpha}_{l+1,m}^{\lambda,\mu}(j,\sigma) - \bar{\alpha}_{l,m}^{\lambda,\mu}(j,\sigma) = \bar{\alpha}_{j+1,m}^{\sigma,\mu}(l,\lambda) - \bar{\alpha}_{j,m}^{\sigma,\mu}(l,\lambda) \tag{49}$$

for $l \neq j, j \pm 1 \vee \lambda \neq \sigma$ and $m \neq j, j+1(l,l+1) \vee \mu \neq \lambda$.

The corresponding boundary phases are

$$\phi_\sigma^{(2)}(\lambda,\mu) = \sum_{j=1}^{L} \bar{\alpha}_{l,m}^{\lambda,\mu}(j,\sigma), \quad \lambda,\mu \neq \sigma, \tag{50}$$

$$\phi_\sigma^{(2)}(\sigma,\mu) = \sum_{\substack{j=1 \\ j \neq l,l-1}}^{L} \bar{\alpha}_{l,m}^{\sigma,\mu}(j,\sigma) + \bar{\alpha}_{l-1,m}^{\sigma,\mu}(l,\sigma) + \bar{\alpha}_{l+1,m}^{\sigma,\mu}(l-1,\sigma), \quad \mu \neq \sigma, \tag{51}$$

$$\phi_\sigma^{(2)}(\sigma,\sigma) = \sum_{\substack{j=1 \\ j \neq l,l\pm 1}}^{L} \bar{\alpha}_{l,l+1}^{\sigma,\sigma}(j,\sigma) + \bar{\alpha}_{l-1,l}^{\sigma,\sigma}(l+1,\sigma) + \bar{\alpha}_{l-1,l+2}^{\sigma,\sigma}(l,\sigma)$$

$$+ \bar{\alpha}_{l+1,l+2}^{\sigma,\sigma}(l-1,\sigma), \tag{52}$$

where $l \neq m, m \pm 1$ can be chosen arbitrarily. The result turns out to be independent of this choice. For less than three sites, [8] Eq. (52) is ill-defined. It reflects a physical limitation: for the boundary phase $\phi_\sigma^{(2)}(\sigma,\sigma)$ to occur, at least three particles with the same spin orientation have to exist; this is possible only if at least three sites are available.

Now we will discuss the effect of the subrelevant parameters $\bar{\alpha}_{j,m}^{\sigma,\mu}(j,\sigma)$ and $\alpha_j^\sigma(j,\sigma)$. The 2-CH subrelevant part of the exponent in the hopping term is $2(\bar{\alpha}_{j,m}^{\sigma,\mu}(j,\sigma) + 3\bar{\xi}_{j,j+1,m}^{\sigma,\sigma,\mu})$. As discussed in the previous section, this term does not vanish in general [9] because the recursive relations do not cover the index grid of $\bar{\xi}$ completely. It contributes to the 1-CH part instead. It has to be added to the right-hand side of Eq. (47). As a consequence, the parameter $\bar{\xi}$ drops out and the recursive relation reads

---

[8] Actually, an equation similar to Eq. (52) but valid for $L \geqslant 4$ only can be obtained by extending Eq. (19) straight forwardly. Eq. (52) has already been suitably extended to its maximum range of validity $L \geqslant 3$, applying the closedness condition Eq. (56).

[9] From the recursive relations, $\bar{\xi}_{j,j+1,\ldots}^{\sigma,\sigma,\ldots}$ expressed in terms of $\bar{\alpha}$ is

$$\bar{\xi}_{1,2,m}^{\sigma,\sigma,\mu}(j,\sigma) := 0$$

$$3\bar{\xi}_{j,j+1,m}^{\sigma,\sigma,\mu}(j,\sigma) = -\sum_{k=2}^{j} \bar{\alpha}_{k-1,m}^{\sigma,\mu}(k,\sigma) + \bar{\alpha}_{k+1,m}^{\sigma,\mu}(k-1,\sigma), \quad j < L,$$

$$3\bar{\xi}_{L,1,m}^{\sigma,\sigma,\mu}(j,\sigma) = -\sum_{k=2}^{L} \bar{\alpha}_{k-1,m}^{\sigma,\mu}(k,\sigma) + \bar{\alpha}_{k+1,m}^{\sigma,\mu}(k-1,\sigma) - \phi_\sigma^{(1)}(\sigma,\mu).$$

But since they drop out of the recursive equations, these relations are not needed here.

$$2\big(\xi_{j,m}^{\sigma,\mu} - \xi_{j+1,m}^{\sigma,\mu}\big) \overset{!}{=} \beta_m^\mu(j,\sigma), \quad m \neq j, j+1 \vee \mu \neq \sigma. \tag{53}$$

where $\beta_m^\mu(j,\sigma)$ is defined as

$$\beta_m^\mu(j,\sigma) := \alpha_m^\mu(j,\sigma) + 2\bar\alpha_{j,m}^{\sigma,\mu}(j,\sigma). \tag{54}$$

Doing the same for the 1-CH subrelevant part in the hopping (concerning Eqs. (48) and (53) now), ζ drops out and in Eq. (48), $\gamma_j(\sigma)$ will be substituted by $\widetilde\gamma_j(\sigma)$

$$\widetilde\gamma_j(\sigma) := \gamma_j(\sigma) + \alpha_j^\sigma(j,\sigma) + 2\bar\alpha_{j,j}^{\sigma,\sigma}(j,\sigma) = \gamma_j(\sigma) + \alpha_j^\sigma(j,\sigma). \tag{55}$$

Using Eq. (53), the second set of closedness conditions are obtained

$$\beta_{m+1}^\mu(j,\sigma) - \beta_m^\mu(j,\sigma) = \beta_{j+1}^\sigma(m,\mu) - \beta_j^\sigma(m,\mu) \tag{56}$$

and the boundary phases are

$$\Phi_\sigma = \phi_\sigma + \sum_\lambda \phi_\sigma^{(1)}(\lambda)(N_\lambda - \delta_{\lambda,\sigma}) + \sum_{\lambda,\mu} \phi_\sigma^{(2)}(\lambda,\mu)(N_\lambda - \delta_{\lambda,\sigma})(N_\mu - \delta_{\mu,\sigma}), \tag{57}$$

where

$$\phi_\sigma^{(1)}(\mu) = \sum_{j=1}^L \beta_m^\mu(j,\sigma), \quad \mu \neq \sigma, \tag{58}$$

$$\phi_\sigma^{(1)}(\sigma) = \sum_{\substack{j=1 \\ j \neq m-1,m}}^L \beta_m^\sigma(j,\sigma) + \beta_{m-1}^\sigma(m,\sigma) + \beta_{m+1}^\sigma(m-1,\sigma), \tag{59}$$

$$\phi_\sigma = \sum_{j=1}^L \widetilde\gamma_j(\sigma). \tag{60}$$

The analysis presented above can be generalized to consider n-CH.

Let $\overset{(n)}{\alpha}, \overset{(n)}{\beta}$ be the parameters of the n-CH part of the hopping:

$$\overset{(n)\{\mathcal{S}\}}{\beta}{}_{\{\mathcal{I}\}}(j,\sigma) := \sum_{k=0}^\infty \binom{n+k}{k} \overset{(n+k)\sigma,\dots,\sigma,\{\mathcal{S}\}}{\alpha}{}_{j,\dots,j,\{\mathcal{I}\}}(j,\sigma) \tag{61}$$

$$= \overset{(n)\{\mathcal{S}\}}{\alpha}{}_{\{\mathcal{I}\}}(j,\sigma) + (n+1)\overset{(n+1)\sigma\{\mathcal{S}\}}{\alpha}{}_{j\{\mathcal{I}\}}(j,\sigma), \tag{62}$$

$$\overset{(n)\sigma,\dots}{\beta}{}_{j,\dots}(j,\sigma) := \overset{(n)\sigma,\sigma,\dots}{\beta}{}_{j,j,\dots}(.,.) := 0. \tag{63}$$

(For multi-chain models the spin index is a multi index spin/chain.) The dots (…) stand for an arbitrary series of indices except they appear in between two equal indices ($\sigma \dots \sigma$). In this case, the void is meant to be filled up with k times σ. $\{\mathcal{S}\}$ is a set of spin- or color indices, $\{\mathcal{I}\}$ a set of coordinate indices. The sum in Eq. (61) of course is finite. The variables are confined since $CL - 1$ is the highest possible correlation level if C is the number of inner degrees of freedom ($C = 2$ for spin 1/2). Hence, $k \leqslant CL - 1 - n$ and for $\bar n$-CH with $\bar n \leqslant CL - 1$, the sum in Eq. (61) already stops at $\bar k = \bar n - n$. Furthermore, as

mentioned above, parameters with coinciding index pairs can be assumed to be zero. This leads to Eq. (62). Eq. (63) only reminds us that all subrelevant parts are removed if β is used instead of α.

The closedness conditions take the form

$$\beta_{l+1,\dots}^{\lambda,\dots}(j,\sigma) - \beta_{l,\dots}^{\lambda,\dots}(j,\sigma) = \beta_{j+1,\dots}^{\sigma,\dots}(l,\lambda) - \beta_{j,\dots}^{\sigma,\dots}(l,\lambda). \tag{64}$$

The n-CH boundary phase is given by

$$\Phi_\sigma^{(n)} = \Phi_\sigma^{(n-1)} + \sum_{\lambda,\dots} \phi_\sigma^{(n)}(\lambda,\dots)(N_\lambda - \delta_{\lambda,\sigma}) \cdots, \tag{65}$$

where the phases $\phi^{(n)}$ are

$$\phi_\sigma^{(n)}(\{\mathcal{S}\}) = \sum_{j=1}^{L} {}^{(n)}\beta_{\{\mathcal{I}\}}^{\{\mathcal{S}\}}(j,\sigma), \quad \sigma \notin \{\mathcal{S}\}, \tag{66}$$

$$\phi_\sigma^{(n)}(\sigma,\dots,\sigma,\{\mathcal{S}'\})$$
$$= \sum_{\substack{j=1 \\ j\neq l_i,l_i-1 \\ i=1,\dots,k}}^{L} {}^{(n)}\beta_{l_1,\dots,l_k,\{\mathcal{I}'\}}^{\sigma,\dots,\sigma,\{\mathcal{S}'\}}(j,\sigma)$$
$$+ \sum_{i=1}^{k} {}^{(n)}\beta_{\dots,l_i-1,\dots,\{\mathcal{I}'\}}^{\sigma,\dots,\sigma,\{\mathcal{S}'\}}(l_i,\sigma) + {}^{(n)}\beta_{\dots,l_i+1,\dots,\{\mathcal{I}'\}}^{\sigma,\dots,\sigma,\{\mathcal{S}'\}}(l_i-1,\sigma) , \quad \sigma \notin \{\mathcal{S}'\}. \tag{67}$$

The pair of index sets $\{\mathcal{S}\}$, $|\{\mathcal{S}\}| = n$ and $\{\mathcal{I}\}$, $|\{\mathcal{I}\}| = n$, respectively $\{\mathcal{S}'\}$, $|\{\mathcal{S}'\}| = n - k$ and $\{\mathcal{I}'\}$, $|\{\mathcal{I}'\}| = n - k$ must not have coinciding index pairs and in Eq. (67) no two l_i must be identical or neighbored. Thus, Eq. (67) holds for $L \geqslant 2k$. This validity range can be maximally enlarged using the closedness conditions (see Eq. (64))

$$\phi_\sigma^{(n)}(\sigma,\dots,\sigma,\{\mathcal{S}'\}) = \sum_{\substack{j=1 \\ j\notin[l,l+k]}}^{L} {}^{(n)}\beta_{l+1,\dots,l+k,\{\mathcal{I}'\}}^{\sigma,\dots,\sigma,\{\mathcal{S}'\}}(j,\sigma) + \sum_{i=0}^{k} {}^{(n)}\beta_{\{\mathcal{L}\}_{i,k},\{\mathcal{I}'\}}^{\sigma,\dots,\sigma,\{\mathcal{S}'\}}(l+i,\sigma),$$
$$\{\mathcal{L}\}_{i,k} = [l, l+k+1] \setminus \{l+i, l+i+1\}, \quad \sigma \notin \{\mathcal{S}'\}. \tag{68}$$

This formula holds for $L \geqslant k + 1$, which is a limit set by physics — analogous to the 2-CH case. The result is l-independent. We point out that $\exp[iF(\{n\})]$ with $F(\{n\})$ being an arbitrary functional of number operators is not the most general unitary operator in Fock space. The most general is $\exp[iG(\{c^\dagger, c\})]$ where $G(\{c^\dagger, c\})$ constitutes a Hermitean functional of the complete set of creation/annihilation operators. In the Appendix C we will show that the class of unitary operators discussed so far is large enough as far as removals of phases in a nearest neighbor hopping term are concerned.

5. Summary and conclusions

In summary, we found a complete characterization of Coordinate Bethe ansatz (CBA) solvable Hubbard-type Hamiltonians with unitary correlated hopping for fermions. A necessary and sufficient criterion for such a Hamiltonian being solvable by CBA was formulated (see Eqs. (9), (10), and (49)).

In contrast to what is suggested in [17], we find that these models are not CBA solvable in the ordinary plane waves basis. Indeed, in such a basis the scattering matrix is configuration dependent (see Appendix A) thus describing diffractive scattering. The particles interact non-trivially even for vanishing Coulomb interaction. Such a situation resembles the case of the impurity problem in the sense that also there, the free picture already contains some residual interaction due to the impurity. Solvability of the models is recovered if the correlations from the hopping terms can be gauged away. This is equivalent to equipping the plane-wave basis with additional density dependent phases. Only in this modified basis can the correlated hopping be absorbed in a boundary term. For the models considered in Refs. [19,20] no such basis exists and hence, they are not solvable by Bethe ansatz as they stand. They can however be repaired by modifying slightly their hopping term, as done at the end of Section 3.

The boundary twists for solvable models with periodic boundary conditions are given explicitly in this work. The corresponding Bethe equations are known from Ref. [16] adapting the boundary phases for a spin degree of freedom only

$$
e^{ip_j L} = e^{-i\Phi_\uparrow} \prod_{a=1}^{N_\downarrow} \frac{i(\sin p_j - \zeta_a) - V/(4t)}{i(\sin p_j - \zeta_a) + V/(4t)},
$$

$$
\prod_{\substack{b=1 \\ b \neq a}}^{N_\downarrow} \frac{i(\zeta_a - \zeta_b) + V/(2t)}{i(\zeta_a - \zeta_b) - V/(2t)} = e^{-i(\Phi_\uparrow - \Phi_\downarrow)} \prod_{l=1}^{N} \frac{i(\sin p_l - \zeta_a) - V/(4t)}{i(\sin p_l - \zeta_a) + V/(4t)}. \tag{69}
$$

Therein, p_j are the quasi-momenta in the plane waves used in the Bethe ansatz (see Eq. (A.1)), ζ_a are spin rapidities, t and V are the Hubbard model parameters and Φ_σ are the boundary phases, which have been determined in this paper. The connection to Ref. [16] shows that in the solvable cases, the correlation in the hopping term of the Hamiltonian (see, for instance, (1)) is equivalent to applying a magnetic flux to the system. However, such a flux is generated by the particles themselves (in particular, it is not an external magnetic flux). Ground state properties can be deduced from those calculated in Refs. [16,23,24]. Even for absent Coulomb interaction, the many particle energy is not a sum of single particle energies. The effect in the energy density is of first order in $1/L$ and in $|\Phi_\uparrow - \Phi_\downarrow|$ in the thermodynamic limit. So one can argue that correlated hopping accounts for a non trivial interaction between the particles even for vanishing Coulomb interaction.

The results obtained here can be applied to models for particles with deformed exchange statistics (DES). This is done via a mapping from DES to CH models [28], whereas special

DES models have been discussed recently using direct Bethe ansatz [23,24]. The details will appear in a forthcoming paper.

Acknowledgements

Appendix A. Configuration dependent S matrix from standard CBA in presence of correlated hopping

In this appendix we explain why correlated hopping destroys solvability by *direct* CBA for Hubbard- and XXZ-type models.

The CBA is an ansatz for the wave function in a so-called fundamental region [25], in which the interaction term doesn't contribute. This fundamental region has to exist at first. For the Hubbard model, this is guaranteed by particle-hole symmetries. This gives the energy in terms of the distinct quasi-momenta. The wave function has to be defined uniquely on the intersection lines of the fundamental regions, where for the Hubbard model also the interaction enters. Both demands yield the S matrix, which represents the effect of the interaction, a scattering of two particles. For Bethe ansatz solvability, the interaction must not have an effect beyond permuting the quasi-momenta of the particles. This demands that the S matrix fulfills the Yang–Baxter equation. Now the boundary conditions, if compatible with the S matrix, lead to additional conditions, fixing the eigenfunctions constructed by Bethe ansatz up to normalization. As a consequence, any additional condition destroys Bethe ansatz solvability. Every correlation in the hopping further restricts the parameters in the Bethe ansatz.

Let us assume a given CH Hubbard-type model can be transformed iso-spectrally to another CH Hubbard-type model, for which fundamental regions exist. This should mean that neither interaction nor correlated hopping contributes. All correlations already contribute, when no interaction is yet to be included. The Bethe ansatz will have the form

$$\psi(x_1, \ldots, x_N) =: \sum_{\pi \in S_N} A(\pi | \pi') e^{i \sum_{k=1}^{N} x_{\pi'(k)} p_{\pi(k)}}, \tag{A.1}$$

where the permutation π' is chosen such that an appropriate order in $(x_1, \ldots, x_N)$ is achieved. Here, the chosen order which defines the fundamental regions, will be: $x_1 \leqslant \cdots \leqslant x_N$.

A.1. "Pinned" correlations

At first assume a correlation which appears if a particle sits at a special site. Let particle number j sit on this site. The effect of this is a shift in all momenta by the correlation strength φ, except that momentum of the designated particle. This is seen by projecting the Schrödinger equation on the specified configuration. The particle causing the correlation with the others feels no correlation from the hopping term applied to it, since it will be transported to that site by the hopping. Thus the resulting term for the energy is

$$E = -2t \sum_{l \neq j}^{N} \cos(p_{\pi(l)} + \varphi) - 2t \cos(p_{\pi(j)}). \tag{A.2}$$

In this equation, π is the momentum permutation from the Bethe ansatz. This energy is neither independent of the permutation as it ought to be, nor does it coincide with the original energy formula $E = -2t \sum_j \cos(p_j)$. Note that φ could even depend on the spin orientation of the considered particles.

A.2. Relative correlations

Assuming the hopping term to be

$$c^{\dagger}_{j+1,\sigma} c_{j,\sigma} \exp(i\varphi n_{j+\Delta,\mu}) + \text{h.c.}, \tag{A.3}$$

where σ and μ are spin indices. Further assume one single particle at coordinate j to be affected by this correlation. The corresponding condition from the Schrödinger equation is

$$\psi(j-1,\sigma; j',\mu)\left(e^{i\varphi n_{j-1+\Delta,\mu}} - 1\right) + \psi(j+1,\sigma; j',\mu)\left(e^{i\varphi n_{j+\Delta,\mu}} - 1\right) = 0, \tag{A.4}$$

where we omitted the spin index from the argument of the wavefunction. Two cases can appear independently from each other:
- a particle with spin orientation μ sits at site $j' = j - 1 + \Delta$,
- a particle with spin orientation μ sits at site $j' = j + \Delta$,

leading to $\psi(j-1,\sigma; j-1+\Delta,\mu) = 0$ in the first case and $\psi(j+1,\sigma; j+\Delta,\mu) = 0$ in the second case. These constraints appear in addition to the usual "continuity" condition arising from $\psi(j,\sigma; j,\mu) = -\psi(j,\sigma; j,\mu)$. If $\sigma = \mu$, at the most two of these three conditions can coincide if $\Delta = 0$ or $\Delta = 1$, which however constitute a subrelevant and irrelevant correlation, respectively. For $\mu = -\sigma$, one of the correlation terms then coincides with the on-site Coulomb interaction. The other, however, is still remaining. The only way out is to modify the Bethe ansatz slightly [26]. In Ref. [26], the fundamental regions are without intersection for different kinds of particles (different spin orientations). Consequently, for different kinds of particles the "continuity" condition is absent and hence substituted by *one* equation coming, e.g., from correlated hopping. The second equation has then to coincide with the interaction. This indicates that the hopping term

$$c^{\dagger}_{j+1,\sigma} c_{j,\sigma} \exp(i\varphi n_{j+\Delta,-\sigma}) + \text{h.c.}, \quad \Delta \in \{0, 1\} \tag{A.5}$$

is the only possible relevant correlated hopping which is tolerable by direct Bethe ansatz for Hubbard-type Hamiltonians (for XXZ-type models no relevant CH is treatable by direct

Bethe ansatz). But then, the obtained S matrix still had to fulfill the Yang–Baxter equation. In Ref. [26], this kind of hopping term is studied. There, φ is purely imaginary and $\Delta(\sigma) := (\sigma + 1)/2 \in \{0, 1\}$ was chosen. This Hamiltonian is shown to be solvable by a modified Bethe ansatz in the absence of Coulomb interaction, $V = 0$. For $V \neq 0$, the resulting S matrix no longer fulfills the Yang–Baxter equation.

To summarize, except for a very special type of relative correlation, namely with particles at distance zero or one towards raising site number, one obtains independent additional sets of conditions which the wave function had to fulfill. This obstructs the direct Bethe ansatz, since the S matrix becomes configuration dependent. It then no longer factorizes into two-particle S matrices. Regarding the exceptional CH mentioned above, a configuration independent S matrix is obtained by applying a variant of Bethe ansatz [26]. But for finite Coulomb interaction strength V, this S matrix does not fulfill the Yang–Baxter equation. As a consequence, no CH XXZ-type model and no interacting CH Hubbard-type model is tractable by direct Bethe ansatz for finite V.

Appendix B. A note on subrelevant parameters

In the following, we will discuss the contribution of the subrelevant parameters. Recalling the definitions, irrelevant parameters like $A_{j-1,j}(\sigma)$ do not at all affect the physics of the model, whereas subrelevant parameters like $A_{j,j}(\sigma)$ contribute to the uncorrelated part of the hopping. For this reason no recursive relations come from them. It is worthwhile noting that Eq. (10) is trivially fulfilled for $m = j$. For this case, the exponent produced after transformation by U is $in_m(2\xi_{j+1,j}^{\sigma,\sigma} + A_{j,j}(\sigma))$. This term hence appears as a phase additional to $\gamma_j(\sigma)$. The parameters $\xi_{j+1,j}^{\sigma,\sigma}$ are (up to an additive constant) given by jumping from 0 to 2 in the exceptional loop in Fig. 1

$$2\big(\xi_{j,j-1}^{\sigma,\sigma} - \xi_{j+1,j}^{\sigma,\sigma} = A_{j,j-1}(\sigma) + A_{j-1,j+1}(\sigma). \tag{B.1}$$

We will now consider the special case in which $2\xi_{j+1,j}^{\sigma,\sigma} + A_{j,j}(\sigma) = 0$ holds. This is exactly what the relation (5) would give for $m = j$. It implies that the subrelevant parameters do not create additional phases in the uncorrelated part of the hopping. Together with (B.1) it gives

$$A_{j,j}(\sigma) - A_{j,j-1}(\sigma) - A_{j-1,j+1}(\sigma) - A_{j-1,j-1}(\sigma) = 0. \tag{B.2}$$

The condition for the relations (5) for $m = j$ and $m = j + 1$ being consistent is $A_{j-1,j} = -A_{j-1,j-1}$, which can always be fulfilled by properly choosing the irrelevant parameter $A_{j-1,j}$. Inserting this into Eq. (B.2), one finally also exactly obtains relation (5) for $m = j + 1$. We can therefore conclude that if Eq. (B.2) holds, the contributions from subrelevant parameters cancel out. It bridges the void in the recursive relations (5).

Since all the α's are relevant, no voids occur in their recursive relations, which is equivalent to all elementary loops being viable.

Appendix C. Unitary transformations in the fermion $u(r)$ algebra

In this appendix, the transformed number operators $c_i^\dagger c_i$ and hopping operators $c_i^\dagger c_j$ will be studied for the most simple unitary transformation such as

$$U = \exp\ i\alpha\big(c_k^\dagger c_l + c_l^\dagger c_k\big) \quad,\quad k \neq l. \tag{C.1}$$

The r^2 operators $\{c_k^\dagger c_l,\ 1 \leqslant i, j \leqslant r\}$ span the Lie algebra $u(r)$:

$$\big[c_i^\dagger c_j, c_k^\dagger c_l\big] = \delta_{j,k} c_i^\dagger c_j - \delta_{i,l} c_k^\dagger c_j, \tag{C.2}$$

where the Cartan basis is generated by $H_i = c_i^\dagger c_i$, $(i = 1, \ldots, r)$:

$$\big[H_i, c_j^\dagger c_k\big] = \big(\delta_{i,j} - \delta_{i,k}\big)\ c_j^\dagger c_k. \tag{C.3}$$

The $u(r)$ algebraic structure allows us to write

$$
\mathrm{e}^{i\alpha \Phi_{k,l}^+} n_m\, \mathrm{e}^{-i\alpha \Phi_{k,l}} = n_m + i\, \Phi_{k,l}^-\big(\delta_{l,m} - \delta_{k,m}\big) - \sin^2\alpha\big(\delta_{l,m} - \delta_{k,m}\big)(n_l - n_k)
$$
$$
+ i(\sin\alpha\cos\alpha - \alpha)\big(\delta_{l,m} - \delta_{k,m}\ \Phi_{k,l}^-,
$$

$$
\mathrm{e}^{i\alpha \Phi_{k,l}^+} \Phi_{m,n}^+\, \mathrm{e}^{-i\alpha \Phi_{k,l}} = \Phi_{m,n}^+ + i\sin\alpha\big[\Phi_{k,n}^-\delta_{l,m} + \Phi_{l,n}^-\delta_{k,m} + \Phi_{k,m}^-\delta_{l,n} + \Phi_{l,m}^-\delta_{k,n}\big]
$$
$$
+ 4\sin\alpha\ \Phi_{k,l}^+\big(\delta_{k,m}\delta_{l,n} + \delta_{l,m}\delta_{k,n}
$$
$$
+ \Phi_{m,n}^+\big(\delta_{k,m} + \delta_{l,n} + \delta_{l,m} + \delta_{k,n}\big)\big], \tag{C.4}
$$

where we applied the following equivalence for adjoints

$$
\mathrm{Ad}\big(\exp(A)\big)\ B := e^A B e^{-A} = \sum_{n=1}^\infty \frac{1}{n!}[A, B]_n =: \exp\ \mathrm{ad}(A)\ B,
$$

$$
[A, B]_0 := B, \quad [A, B]_{n+1} := \big[A, [A, B]_n\big],
$$

and we have defined $\Phi_{k,l}^+ := c_k^\dagger c_l + c_l^\dagger c_k$, and $\Phi_{k,l}^- := c_k^\dagger c_l - c_l^\dagger c_k$ (the Φ^+ are Hermitean, whereas the Φ^- are anti-Hermitean).

From this it is seen that the transformation of the Hubbard Hamiltonian creates arbitrary-range hopping from and to the sites k and l, as well as pair-hopping created from the interaction term. This can be understood from interpreting $\Phi_{k,l}^+$ as a Hamiltonian itself and α as the time. Then, Eq. (C.4) gives the number and hopping operators in the Heisenberg picture. From this interpretation it seems reasonable that no linear combination of $\Phi_{k,l}^+$ with $k \neq l$ will ever be able to just remove phases in a nearest-neighbor hopping term. However, this is not absolutely true. To point out the exceptional cases, the investigation has to be completed. Since the identity $[\mathrm{Ad}(\exp(A))]B = \exp[\mathrm{ad}(A)]B$ does not considerably simplify calculating the action of a more general unitary transformation, another approach will be taken. But at first, the problem will be reduced as far as possible.

In a general product of creation and annihilation operators, one can at first collect operators occurring in pairs using the exchange algebra. The result is a multilinear form of number operators besides a multi-linear form of creation and annihilation operators, so that no two operators have coinciding indices. So the most general exponent appearing in U can be written as follows

$$\xi_{\{p\},\{q\}} \prod_i c^\dagger_{p_i} c_{q_i} + \xi_{k;\{p\},\{q\}} n_k \prod_i c^\dagger_{p_i} c_{q_i} + \xi_{k,l;\{p\},\{q\}} n_k n_l \prod_i c^\dagger_{p_i} c_{q_i} + \cdots . \qquad (C.5)$$

Here, the different ξ are symmetric in the indices before the semicolon and Hermitean in the index sets behind it. They vanish if any two indices coincide. Assuming a pure m-linear form of the creation/annihilation operators, then a transformed bilinear object contains m-linear and even higher terms. This leads to multi-particle hopping and interaction terms including more than two number operators [27]. Since the aim is to stay in the class of Hubbard- or XXZ-type Hamiltonians, we consequently can limit ourselves to general multilinear forms of number operators only, as already studied above, or bilinear forms of creation/annihilation operators only. We will discuss the latter in the following.

$$U := \exp i\xi_{k,l} c^\dagger_k c_l \,, \quad \xi_{k,l} = \xi^*_{l,k}, \ \xi_{k,k} = 0. \qquad (C.6)$$

We point out that $U c^\dagger_m c_n U^{-1}$ is bilinear, since $[c^\dagger_k c_l, c^\dagger_m c_n]$ is bilinear (see C.2). So, one can determine the result by projecting on the desired initial and final states.

$$\langle 0 | c_{m_f} \ \xi_{k,l} c^\dagger_k c_l \ ^n c^\dagger_{m_i} | 0 \rangle$$
$$= \langle 0 | c_{m_f} \ \xi_{k,l} c^\dagger_k c_l \ c^\dagger_{m_{n-1}} | 0 \rangle \langle 0 | c_{m_{n-1}} \cdots c^\dagger_{m_1} | 0 \rangle \langle 0 | c_{m_1} \ \xi_{k,l} c^\dagger_k c_l \ c^\dagger_{m_i} | 0 \rangle$$
$$= \xi_{m_f, m_{n-1}} \xi_{m_{n-1}, m_{n-2}} \cdots \xi_{m_1, m_i} = \left(\xi^n \right)_{m_f, m_i},$$

all written in sum convention. One directly obtains from this

$$\langle 0 | c_{m_f} U c^\dagger_{m_i} | 0 \rangle = (\exp i\xi)_{m_f, m_i}, \qquad (C.7)$$
$$\langle 0 | c_{m_f} U c^\dagger_k c_l U^\dagger c^\dagger_{m_i} | 0 \rangle = (\exp i\xi)_{m_f, k} (\exp i\xi)^*_{m_i, l}, \qquad (C.8)$$

where hermitecity of the ξ was used. The indices k, l are not summed over. It can be shown that the transformed interaction term can never include a single-particle hopping term [27]. This already proves that the reverse direction is also impossible. Thus, number operators and nearest-neighbor hopping have to remain "type-invariant" under the transformation, since the type of Hamiltonian should be preserved. This results in restrictions on the matrix ξ

$$(\exp i\xi)_{m_f, k} (\exp i\xi)^*_{m_i, k} = 0 \quad \forall \, m_f \neq m_i, \qquad (C.9)$$
$$(\exp i\xi)_{m_f, j+1} (\exp i\xi)^*_{m_i, j} = 0 \quad \text{for } |m_f - m_i| > 1. \qquad (C.10)$$

The first conditions emerge from transforming the interaction term, whereas the second one comes from the hopping term. Using both, we can deduce the structure of $\exp i\xi$:

$$(C.9) \implies \forall k \, \exists_1 \, m(k) \ni (\exp i\xi)_{m(k), k} \neq 0,$$
$$(C.10) \implies m(k) = k + \text{const},$$
$$\implies (\exp i\xi)_{k,l}(\Delta) =: \delta_{l, k+\Delta} r_k e^{i\phi_k}, \qquad \prod_k r_l e^{i\phi_l} = 1.$$

Unitarity of the matrix implies $r_l^2 = 1$ for all l. Hence it can be assumed that $r_l = 1$ for all l. So, one finally concludes that $U(\Delta)$ transforms $c^\dagger_{j+1} c_j$ into $c^\dagger_{j+\Delta+1} c_{j+\Delta} e^{i(\phi_{j+1} - \phi_j)}$. Number operators remain unchanged. These phases can be gauged away leaving no

boundary phase. It is worth noting that pure d-range hopping on an L-site chain can also be obtained *iff* d and L are relatively prime. With the analysis used here it can finally be shown that unitary transformations with multinomials of odd degree always produce particle-number violating terms. Hence, they also make us leave the class of models we consider. But it is clear from this, that a huge class of models, which is far from being Hubbard-type can be constructed by unitarily transforming the Hubbard model. They all are solvable and have the same spectrum as the Hubbard model.

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