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Out of equilibrium correlation functions of quantum anisotropic *XY* models: one-particle excitations

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Abstract
We calculate exactly matrix elements between non-equilibrium excitations of the quantum *XY* model for general anisotropy. These matrix elements are expressed as a sum of Pfaffians. For single particle excitations on the ground state, the Pfaffians in the sum simplify to determinants.

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1. Introduction

Spin systems are paradigmatic models for describing many phenomena in contemporary physics [1]. Often, their main properties can be captured qualitatively, resorting to approximated techniques. However, in many cases more refined approaches are required to obtain reliable results. A prime example is systems near or at a phase transition, where quantum fluctuations inhibit many standard routes from working (e.g. mean-field theory but also perturbation theory). At the critical point, in change, the system can be remarkably simplified by a large class of symmetries then present. Conformal field theory systematically employs this important property of the system at criticality and the corresponding dynamics can be integrated exactly in 1+1 dimensions. Many more difficulties arise when the system is far from criticality and accessibility to either mean-field or perturbation theory. Fortunately, there are many non-trivial systems for which the symmetry is large enough to allow the dynamics to be integrated exactly even for generic values of the relevant couplings. Then, the physics of the cross over from non-critical to critical regimes is also accessible. Complete integrability constitutes the crucial property that even exact correlation functions are available. Important steps towards this goal have become possible by the quantum inverse scattering approach [2], more recently refined by Kitanine *et al* [3] and Göhmann and Korepin [4].

The quantum anisotropic *XY* chains are a relevant example of completely integrable models. The model was solved exactly by Lieb *et al* [5] and Pfeuty [6] for isotropic cases and by Barouch *et al* [7] for generic anisotropy. Also, the correlation functions were intensively studied and analytic expressions for their asymptotics (in time and space variables) were obtained [7]. The correlation functions were calculated at equilibrium and for time-dependent magnetic field. We perform an exact calculation of correlations between states that are *not eigenstates* of the model, and this therefore describes *non-equilibrium* properties of the model; we remark that the Hamiltonian instead does not contain explicit time dependence. Our motivation comes from condensed matter where quantum *XY* chains are particularly studied, even more intensively since recent interest in the phenomenon of decoherence in suitably designed physical systems [9]; this latter kind of analysis is due, in turn, to the burst of interest in quantum information theory [10]. Such cross-over of interests led to a line of research investigating the interconnection between condensed matter and quantum information. In particular, it is intriguing to investigate whether it is possible to better characterize condensed matter states by looking at, e.g., quantum correlation *entanglement* properties of their wavefunction [11–20].

The present paper is laid out as follows. In the next section we present the models discussed and review the exact solution from [5, 7], already preparing relevant building blocks for computing off-equilibrium correlations. In section 3 we present known results connecting vacuum expectation values in fermionic theories with a generalized determinant structure, called the Pfaffian and their application to equilibrium correlation functions presented in [6, 7]. Section 4 contains the main result for non-equilibrium correlations and matrix elements of the presented models. After that we draw our conclusions.

2. The models

The system under consideration is a spin-$\frac{1}{2}$ ferromagnetic chain with an exchange coupling λ in a transverse magnetic field of strength h. The Hamiltonian is $H = hH_s$ with the dimensionless Hamilton operator H_s being

$$H_s = -\lambda \sum_{i=1}^{N} (1+\gamma) S_i^x S_{i+1}^x + (1-\gamma) S_i^y S_{i+1}^y - \sum_{i=1}^{N} S_i^z \tag{1}$$

where S^a are the spin-$\frac{1}{2}$ matrices ($a = x, y, z$) and N is the number of sites. We assume periodic boundary conditions. The anisotropy parameter γ connects the quantum Ising model for $\gamma = 1$ with the isotropic *XY* model for $\gamma = 0$. In the interval $0 < \gamma \leqslant 1$ the model belongs to the Ising universality class and for $N = \infty$ it undergoes a quantum phase transition at the critical coupling $\lambda_c = 1$. The order parameter is the magnetization in the x-direction, $\langle S^x \rangle$, which is different from zero for $\lambda > 1$ and vanishes at and below the transition. In contrast the magnetization along the z-direction, $\langle S^z \rangle$, is different from zero for any value of λ.

This class of models was diagonalized by means of the Jordan–Wigner transformation [5–7] that maps spins to one-dimensional spinless fermions with creation and annihilation operators $c_l^\dagger$ and c_l. It proved convenient to use the operators $A_l \doteq c_l^\dagger + c_l$, $B_l \doteq c_l^\dagger - c_l$, which fulfil the anti-commutation rules

$$\{A_l, A_m\} = -\{B_l, B_m\} = 2\delta_{lm} \qquad \{A_l, B_m\} = 0. \tag{2}$$

In terms of these operators the Jordan–Wigner transformation reads

$$S_l^x = \frac{1}{2} A_l \prod_{s=1}^{l-1} A_s B_s \qquad S_l^y = -\frac{\mathrm{i}}{2} B_l \prod_{s=1}^{l-1} A_s B_s \qquad S_l^z = -\frac{1}{2} A_l B_l. \tag{3}$$

The Hamiltonian defined in equation (1) is bilinear in the fermionic degrees of freedom and therefore can be diagonalized by means of the transformation

$$\eta_k = \frac{1}{\sqrt{N}} \sum_l \mathrm{e}^{\mathrm{i}kl} \left(\alpha_k c_l + \mathrm{i}\beta_k c_l^\dagger\right) \tag{4}$$

with coefficients

$$\alpha_k = \frac{\Lambda_k - (1 + \lambda \cos k)}{\sqrt{2\left[\Lambda_k^2 - (1 + \lambda \cos k)\Lambda_k\right]}} \qquad \beta_k = \frac{\gamma \lambda \sin k}{\sqrt{2\left[\Lambda_k^2 - (1 + \lambda \cos k)\Lambda_k\right]}}. \tag{5}$$

The Hamiltonian thereafter assumes the form

$$H = \sum_k \Lambda_k \eta_k^\dagger \eta_k - \frac{1}{2} \sum_k \Lambda_k \tag{6}$$

and the associated energy spectrum is

$$\Lambda_k = \sqrt{(1 + \lambda \cos k)^2 + \lambda^2 \gamma^2 \sin^2 k}.$$

Now, in order to calculate correlations out of equilibrium, we need to know the time dependence of the relevant operators. From equation (4) we obtain the spinless fermion creation and annihilation operators in the Heisenberg scenario. We have $\eta_k^\dagger(t) = \exp(-\mathrm{i}\Lambda_k t)\eta_k^\dagger(0)$ and hence, using equation (4) and its inverse

$$c_j(t) = \sum_l \left[\tilde{a}_{l-j}(t) c_l - \tilde{b}_{l-j}(t) c_l^\dagger\right]$$

where the new coefficients are

$$\tilde{a}_x(t) = \frac{1}{\sqrt{N}} \sum_k \cos kx \left(\mathrm{e}^{\mathrm{i}\Lambda_k t} - 2\mathrm{i}\beta_k^2 \sin \Lambda_k t\right) \tag{7}$$

$$\tilde{b}_x(t) = \frac{2\mathrm{i}}{\sqrt{N}} \sum_k \sin kx \; \alpha_k \; \beta_k \sin \Lambda_k t. \tag{8}$$

In the limit $\gamma = 0$ the previous expressions simplify considerably. In this case the magnetization, i.e. the z-component of the total spin $S^z = \sum_j S_j^z$, is a conserved quantity. In terms of fermions this corresponds to the conservation of the total number of particles, $N = \sum_j n_j = \sum_j c_j^\dagger c_j$. For $\gamma \longrightarrow 0$ and $|\lambda| \leqslant 1$ we find that $\alpha_k \longrightarrow 0$ and $\beta_k \longrightarrow \operatorname{sign} k$. The energy spectrum is $\Lambda_k = |1 + \lambda \cos k|$ and the eigenstates are plane waves (the Hamiltonian corresponds to a tight binding model)

$$c_j(t) = \frac{1}{\sqrt{N}} \sum_k \sum_l \cos k(l - j) \, \mathrm{e}^{-\mathrm{i}\Lambda_k t} c_l \tag{9}$$

$$\eta_k^\dagger = \frac{1}{\sqrt{N}} \sum_l \mathrm{e}^{-\mathrm{i}kl} \, c_l. \tag{10}$$

In this work we discuss vacuum expectation values and correlations in excitations of them. It is worth noting that different strategies are applied, depending on whether the vacuum is the ground state or the state with no particles (which we call the c-vacuum). Since it is cumbersome to calculate the time dependence of the vacuum itself, it is convenient to write the operators A_l and B_l in the Heisenberg scenario. For the ground state instead the time dependence is trivial and the operators are taken in the Schrödinger scenario. For both approaches we express the operators A_l and B_l in terms of the operators η_k and $\eta_k^\dagger$,

$$A_l = \frac{1}{\sqrt{N}} \sum_q \left[\eta_{-q}^\dagger + \eta_q\right] z_q \, \mathrm{e}^{-\mathrm{i}ql} \tag{11}$$

$$B_l = \frac{1}{\sqrt{N}} \sum_q \left[\eta_{-q}^\dagger - \eta_q\right] z_q^* \, \mathrm{e}^{-\mathrm{i}ql}. \tag{12}$$

These are sufficient for the correlations in the ground state. For the calculation for the c-vacuum it proves to be convenient to define the following (redundant) Fourier transforms containing α_k, β_k and their combination $z_k := \alpha_k + \mathrm{i}\beta_k$:

$$\mathfrak{A}_x := \frac{1}{L} \sum_q \mathrm{d}q \, \alpha_q^2 \, \mathrm{e}^{\mathrm{i}qx} \tag{13}$$

$$\mathfrak{B}_x := \frac{1}{L} \sum_q \mathrm{d}q \, \beta_q^2 \, \mathrm{e}^{\mathrm{i}qx} \tag{14}$$

$$\mathfrak{Z}_x := \frac{1}{L} \sum_q \mathrm{d}q \, z_q^2 \, \mathrm{e}^{\mathrm{i}qx} \tag{15}$$

$$\mathfrak{AZ}_x(t) := \frac{1}{L} \sum_q \mathrm{d}q \, \alpha_q z_q \, \mathrm{e}^{\mathrm{i}\Lambda_q t} \, \mathrm{e}^{\mathrm{i}qx} \tag{16}$$

$$\mathfrak{BZ}_x(t) := \frac{1}{L} \sum_q \mathrm{d}q \, \beta_q z_q \, \mathrm{e}^{\mathrm{i}\Lambda_q t} \, \mathrm{e}^{\mathrm{i}qx} \tag{17}$$

$$\mu_x(t) := \mathfrak{AZ}_x^*(t) - \mathrm{i}\mathfrak{BZ}_x(t). \tag{18}$$

In these quantities we have

$$A_l(t) = \sum_j \left(c_j^\dagger \mu_{j-l}(t) + c_j \mu_{j-l}^*(t)\right) \tag{19}$$

$$B_l(t) = \sum_j \left(c_j^\dagger \mu_{l-j}(t) - c_j \mu_{l-j}^*(t)\right) \tag{20}$$

where

$$\mu_x(t) = \frac{1}{L} \sum_q \mathrm{d}q \, \mathrm{e}^{-\mathrm{i}\Lambda_q t} \left(\alpha_q^2 \cos qx + \alpha_q \beta_q \sin qx\right). \tag{21}$$

3. Correlation functions as Pfaffians

It has been known since 1952 that 'vacuum' expectation values of a product of $2R$ fermionic fields

$$\langle 0| \Psi_1 \cdots \Psi_{2R} |0\rangle \tag{22}$$

can be written as a *Pfaffian* [20]. The entries of the Pfaffian structure are the *contractions* of two field operators

$$\langle 0| \Psi_i \Psi_j |0\rangle = P_{i,j}. \tag{23}$$

The field operators Ψ are linear functionals of fermionic creation and annihilation operators, where the 'vacuum' $|0\rangle$ is that state annihilated by the annihilation operators. The Pfaffian is a type of generalized determinant form [20]. It is written in a triangular structure as

$$\sum_{\pi\in\mathcal{S}_{2n}^{<}} (-)^{\pi} P_{\pi(1),\pi(2)} P_{\pi(3),\pi(4)} \cdots P_{\pi(2n-1),\pi(2n)}$$

$$= \begin{vmatrix} P_{1,2} & P_{1,3} & \cdots & P_{1,R} & P_{1,R+1} & P_{1,R+2} & \cdots & P_{1,2R} \\ & P_{2,3} & \cdots & P_{2,R} & P_{2,R+1} & P_{2,R+2} & \cdots & P_{2,2R} \\ & & \cdot & \cdot & \cdot & \cdots & \cdots & \cdot \\ & & & \cdots & \cdot & \cdots & \cdots & \cdot \\ & & & & P_{R,R+1} & P_{R,R+2} & \cdots & P_{R,2R} \\ & & & & & P_{R+1,R+2} & \cdots & P_{R+1,2R} \\ & & & & & & \cdots & \cdot \\ & & & & & & & P_{2R-1,2R} \end{vmatrix} \tag{24}$$

where $\mathcal{S}_{2n}^{<}$ denotes all elements π of the symmetric group $\mathcal{S}_{2n}$ which gives *ordered pairs*; i.e. $\pi(2l-1) < \pi(2l)$ and $\pi(2l-1) < \pi(2m-1)$ for $l < m$. We particularly make use of the known property that a Pfaffian can be expanded along 'rows' or 'columns', where the rth row or column corresponds to all $P_{i,j}$ with $i = r$ or $j = r$. In analogy to matrix minors, we will call the *minor Pfaffian* $\hat{P}_{i,j} \equiv \hat{P}_{j,i}$ the Pfaffian of the above structure (24) when having cancelled the ith and jth rows. In terms of these minors, the expansion reads

$$\mathcal{P}_{2R} = \sum_{\substack{i=1\\ i\neq r}}^{2R-1} (-)^{i+r+1} P_{\overrightarrow{i,r}} \hat{P}_{\overrightarrow{i,r}} \tag{25}$$

where $\overrightarrow{i,r}$ means that the indices are to be written in increasing order. It is worth noting that the rth part of this expansion reflects all possible contractions with the field operator Ψ_r performed in equation (22).

There are two cases which we will study in this work: $|0\rangle$ being (i) the ground state, denoted by $|g\rangle$ and (ii) the c-vacuum, denoted by $|\Downarrow\rangle$.

3.1. Ground state

At equilibrium [5–7], a crucial simplification is that $\langle A_l A_m\rangle_g = -\langle B_l B_m\rangle_g = \delta_{lm}$. This reduces the Pfaffian to a Töplitz determinant

$$\left\langle S_l^{\alpha} S_{l+R}^{\alpha}\right\rangle_g = s(\alpha,\alpha) \begin{vmatrix} 0 & \cdots & 0 & G_{1,1}^{\alpha\alpha} & G_{1,2}^{\alpha\alpha} & \cdots & G_{1,R}^{\alpha\alpha} \\ & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ & & 0 & G_{R-1,1}^{\alpha\alpha} & G_{R-1,2}^{\alpha\alpha} & \cdots & G_{R-1,R}^{\alpha\alpha} \\ & & & G_{R,1}^{\alpha\alpha} & G_{R,2}^{\alpha\alpha} & \cdots & G_{R,R}^{\alpha\alpha} \\ & & & & 0 & \cdots & 0 \\ & & & & & \cdots & \cdots \\ & & & & & & 0 \end{vmatrix}$$

$$= (-)^{R(R-1)/2} s(\alpha,\alpha) \begin{vmatrix} G_{1,1}^{\alpha\alpha} & \cdots & G_{1,R}^{\alpha\alpha} \\ \cdots & \cdots & \cdots \\ G_{R,1}^{\alpha\alpha} & \cdots & G_{R,R}^{\alpha\alpha} \end{vmatrix} \tag{26}$$

with[1]

$$G_{\mu,\nu}^{xx} = \langle A_{l+\mu} B_{l+\nu-1}\rangle_g \tag{27}$$

[1] The link to the notation used in [7] is established by noting that we defined $\mathfrak{Z}_{m-l} = \langle A_l B_m\rangle_g$, which corresponds to the quantity G_{m-l} in [7].

$$G^{yy}_{\mu,\nu} = \langle A_{l+\mu-1} B_{l+\nu} \rangle_g \tag{28}$$

$\langle A_l B_m \rangle_g = \mathfrak{Z}_{m-l}$. The correlation functions $\left\langle S^x_l S^y_{l+R} \right\rangle_g$ and $\left\langle S^y_l S^x_{l+R} \right\rangle_g$ identically vanish, since a complete row and column in the corresponding matrices vanish, respectively. It is worth noting that due to the translational invariance of the state, the determinant above is of Töplitz type. As a consequence the asymptotics of the correlation functions can be extracted explicitly [7] applying the Szegö theorem.

4. Correlation functions out of equilibrium

As already mentioned, time-dependent correlation functions were derived in [7] where the time dependence was explicitly induced into the Hamiltonian (time-dependent external magnetic field). In contrast, we compute matrix elements of operators at non-equilibrium, which means that the initial and final states are not eigenstates of the Hamiltonian; the resulting quantities are then time dependent although the Hamiltonian is not. First, we consider matrix elements in the c-vacuum $|\Downarrow\rangle$ (for generic γ this is not an eigenstate of the Hamiltonian; only for $\gamma = 0$ does it coincide with the ground state), and in excitations on it and on the ground state.

4.1. Correlations in the c-vacuum

Use of equations (19) and (20) leads to the following contractions as building blocks for the Pfaffians:

$$\begin{aligned} \langle A_l(t) B_m(t) \rangle_\Downarrow = \sum_j \mu^*_{j-l} \mu_{m-j} = \delta_{lm} - 4\frac{1}{L} \sum_q \big(2\alpha_q^2 \beta_q^2 \cos q(m-l) \\ + \alpha_q \beta_q \big(1 - 2\beta_q^2\big) \sin q(m-l)\big) \sin^2 \Lambda_q t \end{aligned} \tag{29}$$

$$\langle A_l(t) A_m(t) \rangle_\Downarrow = \sum_j \mu^*_{j-l} \mu_{j-m} = \delta_{lm} - 2\mathrm{i}\frac{1}{L} \sum_q \alpha_q \beta_q \sin q(m-l) \sin 2\Lambda_q t \tag{30}$$

$$\langle B_l(t) B_m(t) \rangle_\Downarrow = \sum_j \mu^*_{j-l} \mu_{l-j} = -\delta_{lm} - 2\mathrm{i}\frac{1}{L} \sum_q \alpha_q \beta_q \sin q(m-l) \sin 2\Lambda_q t. \tag{31}$$

We are now ready to write the two-point spin correlation functions, applying the results from the previous section

$$\begin{aligned} \left\langle S^\alpha_l S^\beta_{l+R} \right\rangle_\Downarrow = s(\alpha,\beta) \\ \times \begin{vmatrix} I^{\alpha\beta}_{1,2} & \cdots & I^{\alpha\beta}_{1,R-1} & J^{\alpha\beta}_1 & F^{\alpha\beta}_1 & G^{\alpha\beta}_{1,2} & \cdot & \cdots & G^{\alpha\beta}_{1,R} \\ & \cdots & \cdots & \cdots & \cdots & \cdots & \cdot & \cdots & \cdots \\ & & I^{\alpha\beta}_{R-2,R-1} & J^{\alpha\beta}_{R-2} & F^{\alpha\beta}_{R-2} & G^{\alpha\beta}_{R-2,2} & \cdot & \cdots & G^{\alpha\beta}_{R-2,R} \\ & & & J^{\alpha\beta}_{R-1} & F^{\alpha\beta}_{R-1} & G^{\alpha\beta}_{R-1,2} & \cdot & \cdots & G^{\alpha\beta}_{R-1,R} \\ & & & & E^{\alpha\beta} & D^{\alpha\beta}_2 & \cdot & \cdots & D^{\alpha\beta}_R \\ & & & & & K^{\alpha\beta}_2 & \cdot & \cdots & K^{\alpha\beta}_R \\ & & & & & & H^{\alpha\beta}_{2,3} & \cdots & H^{\alpha\beta}_{2,R} \\ & & & & & & & \cdots & \cdots \\ & & & & & & & & H^{\alpha\beta}_{R-1,R} \end{vmatrix} \end{aligned} \tag{32}$$

where $s(x,x) = s(y,y) = 1/4(-)^{R(R+1)/2}$,

$$\left.\begin{aligned}
I^{xx}_{\mu,\nu} &= \langle A_{l+\mu}(t) A_{l+\nu}(t)\rangle_{\Downarrow} \\
J^{xx}_{\mu} &= I^{xx}_{\mu,R} \\
H^{xx}_{\mu,\nu} &= \langle B_{l+\mu-1}(t) B_{l+\nu-1}(t)\rangle_{\Downarrow} \\
K^{xx}_{\nu} &= H^{xx}_{1,\nu} \\
G^{xx}_{\mu,\nu} &= \langle A_{l+\mu}(t) B_{l+\nu-1}(t)\rangle_{\Downarrow} \\
F^{xx}_{\mu} &= G^{xx}_{\mu,1} \\
E^{xx} &= G^{xx}_{R,1} \\
D^{xx}_{\nu} &= G^{xx}_{R,\nu}
\end{aligned}\right\} \tag{33}$$

$$\left.\begin{aligned}
I^{yy}_{\mu,\nu} &= \langle A_{l+\mu-1}(t) A_{l+\nu-1}(t)\rangle_{\Downarrow} \\
J^{yy}_{\mu} &= I^{yy}_{\mu,R} \\
H^{yy}_{\mu,\nu} &= \langle B_{l+\mu}(t) B_{l+\nu}(t)\rangle_{\Downarrow} \\
K^{yy}_{\nu} &= H^{yy}_{1,\nu} \\
G^{yy}_{\mu,\nu} &= \langle A_{l+\mu-1}(t) B_{l+\nu}(t)\rangle_{\Downarrow} \\
F^{yy}_{\mu} &= G^{yy}_{\mu,1} \\
E^{yy} &= G^{yy}_{R,1} \\
D^{yy}_{\nu} &= G^{yy}_{R,\nu}
\end{aligned}\right\} \tag{34}$$

and $s(x,y) = s(y,x) = -\mathrm{i}/4(-)^{R(R-1)/2}$,

$$\left.\begin{aligned}
I^{xy}_{\mu,\nu} &= \langle A_{l+\mu}(t) A_{l+\nu}(t)\rangle_{\Downarrow} \\
G^{xy}_{\mu,\nu} &= \langle A_{l+\mu}(t) B_{l+\nu}(t)\rangle_{\Downarrow} \\
J^{xy}_{\mu} &= G^{xy}_{\mu,0} \\
F^{xy}_{\mu} &= G^{xy}_{\mu,1} \\
H^{xy}_{\mu,\nu} &= \langle B_{l+\mu}(t) B_{l+\nu}(t)\rangle_{\Downarrow} \\
E^{xy} &= H^{xy}_{0,1} \\
D^{xy}_{\nu} &= H^{xy}_{0,\nu} \\
K^{xy}_{\nu} &= H^{xy}_{1,\nu}
\end{aligned}\right\} \tag{35}$$

$$\left.\begin{aligned}
I^{yx}_{\mu,\nu} &= \langle A_{l+\mu-1}(t) A_{l+\nu-1}(t)\rangle_{\Downarrow} \\
G^{yx}_{\mu,\nu} &= \langle A_{l+\mu-1}(t) B_{l+\nu-1}(t)\rangle_{\Downarrow} \\
J^{yx}_{\mu} &= I^{yx}_{\mu,R} \\
F^{yx}_{\mu} &= I^{yx}_{\mu,R+1} \\
E^{yx} &= I^{yx}_{R,R+1} \\
D^{yx}_{\nu} &= G^{yx}_{R,\nu} \\
K^{yx}_{\nu} &= G^{yx}_{R+1,\nu} \\
H^{yx}_{\mu,\nu} &= \langle B_{l+\mu-1}(t) B_{l+\nu-1}(t)\rangle_{\Downarrow}
\end{aligned}\right\}. \tag{36}$$

We note that a Pfaffian P can be written (up to a sign) as a determinant of the corresponding antisymmetric matrix A of dimension $2R \times 2R$ [21] by $[pf\,P]^2 = \det A$. Since the c-vacuum is transactional invariant, this determinant is again of Töplitz type. Therefore, also here the asymptotics of the correlation functions could be extracted explicitly along the lines depicted in [7].

4.2. Matrix elements for excitations of the vacuum

We now want to concentrate on expectation values for states which are not the vacuum. So let $\mathcal{C}^\dagger$ and $\mathcal{C}'^\dagger$ be linear functionals in the creation and annihilation operators and let us calculate

$$\langle \mathcal{C}|\, \Psi_1 \cdots \Psi_{2R} |\mathcal{C}'\rangle := \langle 0|\, \mathcal{C}\Psi_1 \cdots \Psi_{2R}\mathcal{C}'^\dagger |0\rangle. \tag{37}$$

Performing all possible contractions in (37), we obtain $\langle 0|\,\mathcal{C}\mathcal{C}'^\dagger\,|0\rangle\,\langle 0|\,\Psi_1 \cdots \Psi_{2R}\,|0\rangle$ plus all possible contractions where $\mathcal{C}$ and $\mathcal{C}'^\dagger$ are contracted with a pair of field operators, say Ψ_i and Ψ_j. Thus, we have to calculate

$$\tilde{P}_{i,j} := \langle \mathcal{C}|\Psi_i|0\rangle\langle 0|\Psi_j|\mathcal{C}'\rangle - \langle \mathcal{C}|\Psi_j|0\rangle\langle 0|\Psi_i|\mathcal{C}'\rangle \tag{38}$$

where we take $i < j$ in order to avoid double counting of contractions. The sign coming from the transportation of the operators $\mathcal{C}$ and $\mathcal{C}'^\dagger$ to the left of Ψ_i and the right of Ψ_j respectively is $(-)^{i+j+1}$. In the remaining vacuum expectation value, the field operators Ψ_i and Ψ_j are missing, which corresponds to the cancellation of the rows i and j in the original Pfaffian (24). Consequently, this expectation value is the minor Pfaffian $\hat{P}_{\overrightarrow{i,j}}$, and we obtain

$$\begin{aligned}\langle \mathcal{C}|\, \Psi_1 \cdots \Psi_{2R}|\mathcal{C}'\rangle &:= \mathcal{P}_{2R} + \sum_{i=1}^{2R-1}\sum_{j=i+1}^{2R} (-)^{i+j+1}\,\tilde{P}_{i,j}\,\hat{P}_{\overrightarrow{i,j}} \\ &= \mathcal{P}_{2R} + \sum_{i=1}^{2R-1}\left(\sum_{j=1}^{i-1}(-)^{i+j+1}0\cdot \hat{P}_{\overrightarrow{i,j}} + \sum_{j=i+1}^{2R}(-)^{i+j+1}\,\tilde{P}_{i,j}\,\hat{P}_{\overrightarrow{i,j}}\right).\end{aligned}$$

We note that this expression is the sum over Pfaffian expansions (25). Indeed, each element of the first sum is the expansion of a Pfaffian along the ith row, in which $P_{j,i} = 0$ and $P_{i,j} \to \tilde{P}_{i,j}$, hence

$$\langle \mathcal{C}|\, \Psi_1 \cdots \Psi_{2R}|\mathcal{C}'\rangle := \sum_{i=0}^{2R-1} \mathcal{P}_{2R}^{(i)} \tag{39}$$

where we defined

$$\mathcal{P}_{2R}^{(0)} := \mathcal{P}_{2R}$$

and

$$\mathcal{P}_{2R}^{(i)} := \left|\begin{array}{cccccc} P_{1,2} & \cdots & 0 & P_{1,i+1} & \cdots & P_{1,2R} \\ & \cdots & \cdots & \cdots & \cdots & \cdots \\ & & 0 & P_{i-1,i+1} & \cdots & P_{i-1,2R} \\ & & & \tilde{P}_{i,i+1} & \cdots & \tilde{P}_{i,2R} \\ & & & & \cdots & \cdots \\ & & & & & P_{2R-1,2R} \end{array}\right|. \tag{40}$$

Actually, we found the correlations $\langle \mathcal{C}|S_l^\alpha S_m^\beta|\mathcal{C}'\rangle$ expressed as a *sum of* Pfaffians. The generalization to operators $\mathcal{C}^\dagger$ that are multi-linear in the annihilation and creation operators can be related to a sum of multi-row expanded Pfaffians [22].

In what follows, we will come back to the cases of the ground state and the c-vacuum, discussed in the previous section. As mentioned, in order to explicitly extract the asymptotics of the correlations, the initial and final states have to be transactional invariant. In the following, the translational invariance is explicitly broken.

4.2.1. Single hole excitations on the ground state. We choose the final and initial states to be $\langle \mathcal{C}| = \langle g|\, c_j^\dagger \big/ \sqrt{\mathfrak{B}_0} =: \langle j|$ and $|\mathcal{C}'\rangle = c_k|g\rangle/\sqrt{\mathfrak{B}_0} =: |k\rangle$, which are normalized due to $\langle g|\, c_j^\dagger c_k\,|g\rangle = \mathfrak{B}_{k-j}$. Then we calculate

$$\langle A_l B_m\rangle_g^{jk} \doteq \langle j|A_l|g\rangle\langle g|B_m|k\rangle - \langle j|B_m|g\rangle\langle g|A_l|k\rangle.$$

In this case we find

$$\langle A_l B_m\rangle_g^{jk} = \frac{\mathfrak{B}\mathfrak{Z}_{j-l}\mathfrak{B}\mathfrak{Z}^*_{m-k} + \mathfrak{B}\mathfrak{Z}_{m-j}\mathfrak{B}\mathfrak{Z}^*_{k-l}}{\mathfrak{B}_0} \tag{41}$$

$$\langle A_l A_m\rangle_g^{jk} = \frac{\mathfrak{B}\mathfrak{Z}^*_{k-m}\mathfrak{B}\mathfrak{Z}_{j-l} - \mathfrak{B}\mathfrak{Z}^*_{k-l}\mathfrak{B}\mathfrak{Z}_{j-m}}{\mathfrak{B}_0} \tag{42}$$

$$\langle B_l B_m\rangle_g^{jk} = -\frac{\mathfrak{B}\mathfrak{Z}^*_{m-k}\mathfrak{B}\mathfrak{Z}_{l-j} - \mathfrak{B}\mathfrak{Z}^*_{l-k}\mathfrak{B}\mathfrak{Z}_{m-j}}{\mathfrak{B}_0}. \tag{43}$$

The contraction of $\mathcal{C}$ with $\mathcal{C}'$ is

$$\langle 0|\,\mathcal{C}\mathcal{C}'|0\rangle = \frac{\mathfrak{B}_{k-j}}{\mathfrak{B}_0}. \tag{44}$$

We now discuss the correlation functions $\left\langle S_l^\alpha S_{l+R}^\alpha\right\rangle$. The only non-zero contributions come from contractions of $\mathcal{C}$ and $\mathcal{C}'$ with one operator of type A and one of type B (since only vacuum expectations of an equal number of As and Bs are non-zero as discussed before). This means that here the sum of Pfaffians simplifies to the following sum of determinants:

$$\left\langle S_l^\alpha S_l^\alpha\right\rangle = \sum_{i=1}^{R} \mathcal{D}_R^{(i)}$$

with

$$\mathcal{D}_R^{(i)} = (-1)^R \begin{vmatrix} G^{\alpha\alpha}_{1,1} & \cdots & G^{\alpha\alpha}_{1,R} \\ \cdots & \cdots & \cdots \\ \tilde{G}^{\alpha\alpha}_{i,1} & \cdots & \tilde{G}^{\alpha\alpha}_{i,R} \\ \cdots & \cdots & \cdots \\ G^{\alpha\alpha}_{R,1} & \cdots & G^{\alpha\alpha}_{R,R} \end{vmatrix} \tag{45}$$

with

$$G^{xx}_{\mu,\nu} = \langle A_{l+\mu} B_{l+\nu-1}\rangle_g \tag{46}$$

$$\tilde{G}^{xx}_{\mu,\nu} = \langle A_{l+\mu} B_{l+\nu-1}\rangle_g^{jk} \tag{47}$$

$$G^{yy}_{\mu,\nu} = \langle A_{l+\mu-1} B_{l+\nu}\rangle_g \tag{48}$$

$$\tilde{G}^{yy}_{\mu,\nu} = \langle A_{l+\mu-1} B_{l+\nu}\rangle_g^{jk}. \tag{49}$$

Analogously, for the correlation functions $\left\langle S_l^x S_{l+R}^y\right\rangle$ and $\left\langle S_l^y S_{l+R}^x\right\rangle$, the only non-zero contributions come from contractions of $\mathcal{C}$ and $\mathcal{C}'$ with two operators of type B and two of type A, respectively. This again simplifies the sum of Pfaffians to a sum of determinants

$$\left\langle S_l^x S_l^y\right\rangle = \sum_{i=1}^{R} \mathcal{P}_{2R}^{(i)}$$

where

$$\mathcal{P}_{2R}^{(i)} = \left| \begin{array}{ccccccccccc}
0 & \cdots & 0 & G^{xy}_{1,1} & \cdot & \cdots & 0 & G^{xy}_{1,i+1} & \cdot & \cdots & G^{xy}_{1,R+1} \\
 & \cdots & \cdot & \cdots & \cdot & \cdots & \cdot & \cdot & \cdot & \cdots & \cdot \\
 & & 0 & G^{xy}_{R-2,1} & \cdot & \cdots & \cdot & G^{xy}_{R-2,i+1} & \cdot & \cdots & \cdot \\
 & & & G^{xy}_{R-1,1} & \cdot & \cdots & 0 & G^{xy}_{R-1,i+1} & \cdot & \cdots & G^{xy}_{R-1,R+1} \\
 & & & & 0 & \cdots & 0 & 0 & \cdot & \cdots & 0 \\
 & & & & & \cdots & \cdot & \cdot & \cdot & \cdots & \cdot \\
 & & & & & & 0 & 0 & \cdot & \cdots & 0 \\
 & & & & & & & \tilde{H}^{xy}_{i,i+1} & \cdot & \cdots & \tilde{H}^{xy}_{i,R+1} \\
 & & & & & & & & 0 & \cdots & 0 \\
 & & & & & & & & & \cdots & \cdot \\
 & & & & & & & & & & 0
\end{array} \right| \tag{50}$$

and this simplifies to

$$\left\langle S_l^x S_l^y \right\rangle = \sum_{i=1}^{R} \mathcal{D}_R^{(i)}$$

with

$$\mathcal{D}_R^{(i)} = (-1)^R \left| \begin{array}{cccccc}
G^{xy}_{1,1} & \cdots & G^{xy}_{1,i-1} & G^{xy}_{1,i+1} & \cdots & G^{xy}_{1,R+1} \\
\cdots & \cdots & \cdots & \cdots & \cdots & \\
G^{xy}_{R-1,1} & \cdots & G^{xy}_{R-1,i-1} & G^{xy}_{R-1,i+1} & \cdots & G^{xy}_{R-1,R+1} \\
0 & \cdots & 0 & \tilde{H}^{xy}_{i,i+1} & \cdots & \tilde{H}^{xy}_{i,R+1}
\end{array} \right| \tag{51}$$

with

$$G^{xy}_{\mu,\nu} = \langle A_{l+\mu} B_{l+\nu-1} \rangle_g \tag{52}$$

$$\tilde{H}^{xy}_{\mu,\nu} = \langle B_{l+\mu-1} B_{l+\nu-1} \rangle_g^{jk}. \tag{53}$$

In an analogous way we find

$$\left\langle S_l^y S_l^x \right\rangle = \sum_{i=1}^{R} \mathcal{D}_R^{(i)}$$

with $\mathcal{D}_R^{(i)}$ defined as in (51), but

$$G^{xy}_{\mu,\nu} = \langle A_{l+\nu-1} B_{l+\mu} \rangle_g \tag{54}$$

$$\tilde{H}^{xy}_{\mu,\nu} = \langle A_{l+\mu-1} A_{l+\nu-1} \rangle_g^{jk}. \tag{55}$$

4.2.2. Single particle excitations in the ground state. Alternatively, we consider $\langle \mathcal{C}| = \langle g|\, c_j/\sqrt{\mathfrak{A}_0} =: \langle j|$ and $|\mathcal{C}'\rangle = c_k^\dagger |g\rangle/\sqrt{\mathfrak{A}_0} =: |k\rangle$ as final and initial states, which are again normalized according to $\langle g|\, c_j^\dagger c_k\, |g\rangle = \mathfrak{A}_{k-j}$. In this case the possible contractions with the operators $\mathcal{C}$ and $\mathcal{C}'$ are

$$\langle A_l B_m \rangle_g^{jk} = -\frac{\mathfrak{A}\mathfrak{Z}_{k-l}\mathfrak{A}\mathfrak{Z}^*_{m-j} + \mathfrak{A}\mathfrak{Z}_{m-k}\mathfrak{A}\mathfrak{Z}^*_{j-l}}{\mathfrak{A}_0} \tag{56}$$

$$\langle A_l A_m \rangle_g^{jk} = \frac{\mathfrak{A}\mathfrak{Z}^*_{j-m}\mathfrak{A}\mathfrak{Z}_{k-l} - \mathfrak{A}\mathfrak{Z}^*_{j-l}\mathfrak{A}\mathfrak{Z}_{k-m}}{\mathfrak{A}_0} \tag{57}$$

$$\langle B_l B_m \rangle_g^{jk} = -\frac{\mathfrak{A}\mathfrak{Z}^*_{m-j}\mathfrak{A}\mathfrak{Z}_{l-k} - \mathfrak{A}\mathfrak{Z}^*_{l-j}\mathfrak{A}\mathfrak{Z}_{m-k}}{\mathfrak{A}_0}. \tag{58}$$

The contraction of $\mathcal{C}$ with $\mathcal{C}'$ is here

$$\langle 0| \mathcal{C}\mathcal{C}' |0\rangle = \frac{\mathfrak{A}_{k-j}}{\mathfrak{A}_0}. \tag{59}$$

4.2.3. Single particle excitations in the c-vacuum. We take the final and initial states to be $\langle\mathcal{C}| = \langle 0| c_j =: \langle j|$ and $|\mathcal{C}'\rangle = c_k^\dagger =: |k\rangle$. In this case the Pfaffian $\mathcal{P}^i_{2R}$ is given by equations (32)–(36), where (following equation (40)) in the ith row

$$\langle\Downarrow| A_l B_m |\Downarrow\rangle \longrightarrow \langle A_l B_m \rangle_\Downarrow^{jk}$$

are replaced with

$$\langle A_l B_m \rangle_\Downarrow^{jk} \doteq \langle j|A_l|\Downarrow\rangle\langle\Downarrow|B_m|k\rangle - \langle j|B_m|\Downarrow\rangle\langle\Downarrow|A_l|k\rangle$$

and in the same manner $\langle\Downarrow|A_l A_m|\Downarrow\rangle \longrightarrow \langle A_l A_m\rangle_\Downarrow^{jk}$, $\langle\Downarrow|B_l B_m|\Downarrow\rangle \longrightarrow \langle B_l B_m\rangle_\Downarrow^{jk}$. We find

$$\langle A_l(t) B_m(t)\rangle_\Downarrow^{jk} = -(\mu_{m-j}\mu^*_{k-l} + \mu_{j-l}\mu^*_{m-k}) \tag{60}$$

$$\langle A_l(t) A_m(t)\rangle_\Downarrow^{jk} = \mu_{j-l}\mu^*_{k-m} - \mu_{j-m}\mu^*_{k-l} \tag{61}$$

$$\langle B_l(t) B_m(t)\rangle_\Downarrow^{jk} = \mu_{m-j}\mu^*_{l-k} - \mu_{l-j}\mu^*_{m-k}. \tag{62}$$

With these results, all spin-correlation functions can be calculated as long as $\langle\mathcal{C}| S_l^x(t = 0)|\mathcal{C}'\rangle = \langle\mathcal{C}| S_l^y(t = 0)|\mathcal{C}'\rangle = 0$. In this case it will remain zero during the evolution. This is satisfied if the parity symmetry of the Hamiltonian is broken neither by the initial nor by the final state.

5. Conclusions

We calculated exactly spin–spin correlations out of equilibrium. For excitations on the 'vacuum', they can be written as a sum of Pfaffians. For excitations on the ground state these Pfaffians reduce to determinants (see equations (39) and (40)). The results for particle and hole excitations on the ground state and the c-vacuum were based on different approaches, writing the fermionic field operators in the Schrödinger and Heisenberg scenarios, respectively. Comparing with the known eigenstate correlations, we remark that here $\left\langle S_l^\alpha S_{l+R}^\alpha \right\rangle$ cannot be reduced to $R \times R$ Töplitz determinants. For the vacuum-correlation functions the Pfaffians instead can be related to $2R \times 2R$ Töplitz determinants. For correlation functions in excited states (of the vacuum), the translational invariance of the system is explicitly broken and then the determinants are no longer of Töplitz type. The last issue constitutes a further difficulty of the problem of finding the asymptotics of the correlations since the Szegö theorem cannot be applied.

We have used these results explicitly for studying the dynamics of correlations and quantum information theoretic quantities such as the entanglement in specific states [19] but is also a key ingredient for the study of transport properties of the system. One possible application of the exact results we found here is to study the quantum phase transitions (characteristic of this class of models) out of equilibrium.

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