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Hierarchy of double-time correlations

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Abstract. The hierarchy of correlations is an approximation scheme which permits the study of non-equilibrium phenomena in strongly interacting quantum many-body systems on lattices in higher dimensions (with the underlying idea being somewhat similar to dynamical mean-field theory). So far, this method was restricted to equal-time correlators such as $\langle \hat{A}_{\mu}(t)\hat{B}_{\nu}(t)\rangle$. Using the method of complete induction, we generalize this method to double-time correlators such as $\langle \hat{A}_{\mu}(t)\hat{B}_{\nu}(t')\rangle$. The hierarchical decoupling scheme permits the evaluation of correlation functions in thermal equilibrium as well as in non-equilibrium settings. As an application, we study the equilibrium dynamics of correlation functions and the related light-cone structure of the bosonic Hubbard model in the Mott insulator phase. Furthermore we address the light-cone structure when the system is quenched.

Keywords: strongly correlated systems, hierarchy of correlations, Bose Hubbard model, finite temperature Green's functions, quantum quenches

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1. Introduction

The physics of strongly interacting quantum many-body systems is, despite decades of research, far from being fully understood. Apart from a few exactly solvable models, even their ground state properties are a subject of ongoing discussions, see, e.g. [1, 2]. Even more challenging is the investigation of non-equilibrium properties of those interacting many-body systems.

In the limit of infinite dimensions, the dynamical mean-field theory (DMFT) has been successfully applied to various problems such as the Mott–Hubbard transition [3–8] or the non-equilibrium dynamics in Mott insulators [9–14] by mapping the system to an effective single site (i.e. zero-dimensional) problem.

Furthermore, one-dimensional strongly interacting systems have been studied by employing exact diagonalization, see, e.g. [15–24], time-dependent density matrix renormalization group variational techniques (t-DMRG), see, e.g. [25–27], or Jordan–Wigner transformations [28–31]. Moreover, exact analytical solutions were used to study nonequilibrium dynamics [32] and ground state properties. However, the findings for onedimensional systems cannot be easily transferred to higher dimensions. For example, thermalization in higher dimensions is very different from thermalization in one dimension since for the latter the energy re-distribution cannot occur via two-body collisions (due to energy and momenta conservation).

For strongly interacting systems in higher dimensions, the methods described above run into difficulties. For example, the generalization of t-DMRG to higher dimensions (such as tensor networks) is limited by the exponential scaling with the system size [33],

especially if correlations spread across the system. For a very similar reason (exponential scaling of Hilbert space), the method of exact diagonalization is limited to small system sizes [15–24]. On the other hand, the DMFT is only well controlled in the limit of infinite dimensions and, due to the mapping to an effective single-site problem, does not capture energy and momentum transfer of quasi-particles or long-range correlations, see, e.g. [34].

As an extension of the DMFT methods, various cluster approaches have been developed which capture all correlations within a finite range (cluster). The coupling of the cluster to the surrounding lattice can, for example, be included via a self-consistent embedding in a mean-field, see, e.g. [35, 36]. These cluster extensions of the DMFT method provide a controlled way of approaching the exact limit by increasing the cluster size.

In order to take correlations of arbitrarily long range into account, we established over the last years a perturbative hierarchical method which is valid for large coordination numbers $Z \gg 1$.

Somewhat complementary to the cluster approach, our method captures two-site correlations of arbitrary range to first order in 1/Z whereas higher-order correlations among more than two lattice sites are included at higher orders in 1/Z. This method allows for a systematic study of non-equilibrium properties in strongly interacting systems in large (but finite) dimensions.

The hierarchical expansion is based on a controlled expansion of the n-point reduced density matrices into correlated parts. At zeroth order in our expansion, we have the single-site density matrix,

$$\hat{\rho}_{\mu} = \operatorname{Tr}_{\mu}\{\hat{\rho}\} = \mathcal{O}(Z^0), \qquad (1)$$

where Tr_{μ} denotes the trace over all lattice sites but μ . The correlated part of the two-site density matrix,

$$\hat{\rho}_{\mu\nu}^{\text{corr}} = \text{Tr}_{\mu\nu} \{\hat{\rho}\} - \hat{\rho}_{\mu} \hat{\rho}_{\nu} = \mathcal{O}(1/Z), \qquad (2)$$

scales linearly in 1/Z, the three-point correlator

$$\hat{\rho}_{\mu\nu\lambda}^{\text{corr}} = \text{Tr}_{\mu\nu\lambda} \{\hat{\rho}\} - \hat{\rho}_{\mu\nu}^{\text{corr}} \hat{\rho}_{\lambda} - \hat{\rho}_{\mu\lambda}^{\text{corr}} \hat{\rho}_{\nu} - \hat{\rho}_{\nu\lambda}^{\text{corr}} \hat{\rho}_{\lambda} - \hat{\rho}_{\mu} \hat{\rho}_{\nu} \hat{\rho}_{\lambda} = \mathcal{O}(1/Z^2)$$
(3)

scales quadratically, and so on. The time-evolution of the n-point correlations is derived directly from the von Neumann equations.

The above scaling with powers of 1/Z facilitates a controlled iterative approximation scheme. The zeroth order $\mathcal{O}(Z^0)$ can be used to infer the mean-field background. Perturbations around this mean-field background can be treated within first order in 1/Zand yield the quasi-particle excitations and their spectra, etc. Iterating this approximation scheme further, one may include the back-reaction of the quasi-particle fluctuations onto the mean-field or derive the interactions between the quasi-particles, etc.

With this expansion, we were able to study quenches across phase boundaries [37], ground state properties and non-equilibrium dynamics of quantum correlations in the bosonic and fermionic Hubbard model [38, 39], an analogue for the Sauter–Schwinger

effect [40], phase boundaries [41] and the Boltzmann dynamics of quasi-particle excitations in strongly interacting systems [42–46].

The derivation of the hierarchy (1)-(3) was based on the real-time evolution of the system's density matrix. In the following, we shall extend our hierarchical approach to double-time correlation functions. As a concrete example, we will apply the method to the Bose–Hubbard model in the Mott insulating phase.

As will be shown in section 4, the hierarchy for two-time correlation functions can also be used for double-time Green's functions. In this context, various decoupling schemes have been developed and applied, for example, to spin models [47–52] or interacting many-particle systems [53–57]. These decoupling schemes reside on the disregard of spin fluctuations or correlations among particles. Here we use a decoupling scheme which is based on the truncation of correlations among lattice sites. The small expansion parameter 1/Z is employed to derive the (truncated) hierarchical equations at a given order and to specify the error of the decoupling procedure.

2. The double-time hierarchy

We consider quantum many-body systems on a lattice as described by the general Hamiltonian

$$\hat{H} = -\frac{J}{Z} \sum_{\mu,\nu} T_{\mu\nu} \hat{X}^{\dagger}_{\mu} \hat{X}_{\nu} + \sum_{\mu} \hat{H}_{\mu}.$$
(4)

Here μ and ν denote lattice sites while \hat{H}_{μ} and \hat{X}_{ν} are local (on-site) operators acting on the local Hilbert spaces associated to those sites. Here, we consider one set of operators \hat{X}_{μ} only, but it is straight-forward to include multiple sets $\hat{X}_{\mu,s}$ labeled by the additional quantum number s which could be the spin, for example.

The lattice structure is encoded in the adjacency matrix $T_{\mu\nu}$ where Z is the coordination number, which is assumed to be large $Z \gg 1$. Finally, J denotes the coupling strength between neighboring lattice sites, see the next section for an explicit example.

As a generalization of the hierarchy of correlations in equations (1)–(3) above, we consider expectation values of operators at two different times t and t'. For two operators $\hat{A}_{\mu}(t)$ and $\hat{B}_{\mu}(t)$ acting on the same lattice site, the generalization of equation (1) above reads

$$\langle \hat{A}_{\mu}(t)\hat{B}_{\mu}(t')\rangle = \mathcal{O}(Z^0).$$
(5)

Here we define the time-dependent expectation values of the operators as usual via $\langle \ldots \rangle = \operatorname{tr}(\ldots \hat{\rho})$ where $\hat{\rho}$ denotes the full density matrix of the total lattice in the Heisenberg representation.

Considering two operators $\hat{A}_{\mu}(t)$ and $\hat{B}_{\nu}(t')$ acting on different lattice sites, we may define their correlations in the usual way. The central point is that these two-point correlators are also suppressed as $\mathcal{O}(1/Z)$, i.e. the generalization of equation (2) reads [58]

$$\langle \hat{A}_{\mu}(t)\hat{B}_{\nu}(t')\rangle^{\text{corr}} = \langle \hat{A}_{\mu}(t)\hat{B}_{\nu}(t')\rangle - \langle \hat{A}_{\mu}(t)\rangle\langle \hat{B}_{\nu}(t')\rangle = \mathcal{O}(1/Z).$$
(6)

In analogy to equation (3), this can be extended to higher-order correlations. The most general double-time expectation value has the form $\langle \hat{A}_{\mathcal{S}}(t)\hat{B}_{\mathcal{S}}(t')\rangle$ where \mathcal{S} denotes the set of $|\mathcal{S}|$ lattice sites. For example, for $\mathcal{S} = \{\mu, \nu\}$, we have $|\mathcal{S}| = 2$ and we may set $\hat{A}_{\mathcal{S}}(t) = \hat{A}_{\mu}(t) \otimes \mathbf{1}_{\nu}$ and $\hat{B}_{\mathcal{S}}(t') = \hat{B}_{\nu}(t) \otimes \mathbf{1}_{\mu}$.

Separating the expectation value $\langle \hat{A}_{\mathcal{S}}(t)\hat{B}_{\mathcal{S}}(t')\rangle$ involving $|\mathcal{S}|$ lattice sites into the product of the local on-site expectation values plus the correlations of second and higher order, up to the order $|\mathcal{S}|$, we find that these correlators are suppressed according to

$$\langle \hat{A}_{\mathcal{S}}(t)\hat{B}_{\mathcal{S}}(t')\rangle^{\text{corr}} = \mathcal{O}(Z^{1-|\mathcal{S}|}).$$
(7)

As we show in the appendix using the method of complete induction, the evolution equations for these correlators conserve this hierarchy (7). Thus, assuming an initial state $\hat{\rho}$ which respects this hierarchy (7), it remains valid for finite times t and t'. One option is to envisage an initial thermal equilibrium state for a disconnected lattice J = 0where all correlations between lattice sites vanish. Then, by slowly switching on J(t), we may induce correlations while still staying close to thermal equilibrium, but these correlators must respect the hierarchy (7).

Employing this hierarchy (7), we may again develop a consistent approximation scheme based on an expansion into powers of 1/Z. In the next sections, we discuss such a scheme for the prototypical example of the Bose–Hubbard model.

3. The Bose–Hubbard model

The lattice system under consideration is described by the Bose–Hubbard Hamiltonian $(\hbar=1)$

$$\hat{H} = -\frac{J(t)}{Z} \sum_{\mu,\nu} T_{\mu\nu} \hat{b}^{\dagger}_{\mu} \hat{b}_{\nu} + \sum_{\mu} \left[\frac{U}{2} \hat{n}_{\mu} (\hat{n}_{\mu} - 1) - \mu_0 \hat{n}_{\mu} \right]$$
(8)

with the bosonic creation and annihilation operators \hat{b}^{\dagger}_{μ} and \hat{b}_{ν} and the particle number operator $\hat{n}_{\mu} = \hat{b}^{\dagger}_{\mu}\hat{b}_{\mu}$. The kinetic term is determined by the time-dependent hopping rate J(t) and the coordination number Z. All bosons are subject to a on-site repulsion U if a lattice site is occupied with more than one particle. The number operator is denoted with \hat{n}_{μ} and μ_0 is the chemical potential.

We assume the system to be in the Mott insulating phase where the on-site repulsion U dominates over the hopping rate J. To order $\mathcal{O}(Z^0)$, the density matrix of the system is given by

$$\hat{\rho} = \bigotimes_{\mu} \hat{\rho}_{\mu}, \quad \hat{\rho}_{\mu} = \sum_{n} p_{n}(t) |n\rangle_{\mu} \langle n|$$
(9)

with the on-site probabilities $p_n(t)$. In the following, we use the operators $\hat{P}^{n,m}_{\mu} = |n\rangle_{\mu} \langle m|$ which are sometimes referred to as Hubbard operators [59]. We find for the on-site expectation values

$$(i\partial_t - Un + \mu_0) \langle \hat{P}^{n,n+1}_{\mu}(t) \hat{P}^{m+1,m}_{\mu}(t') \rangle = \mathcal{O}(1/Z).$$
(10)

The two-site correlation functions with $\mu \neq \nu$ evolve according to

$$(i\partial_{t} - Un + \mu_{0}) \langle \hat{P}_{\mu}^{n,n+1}(t) \hat{P}_{\nu}^{m+1,m}(t') \rangle^{\text{corr}} = -\frac{J(t)}{Z} \sum_{\kappa \neq \mu,\nu} T_{\mu\kappa} \sqrt{n+1} [p_{n}(t) - p_{n+1}(t)] \langle \hat{b}_{\kappa}(t) \hat{P}_{\nu}^{m+1,m}(t') \rangle^{\text{corr}} - \frac{J(t)}{Z} T_{\mu\nu} \sqrt{n+1} [p_{n}(t) - p_{n+1}(t)] \langle \hat{b}_{\nu}(t) \hat{P}_{\nu}^{m+1,m}(t') \rangle + \mathcal{O}(1/Z^{2}).$$
(11)

In equation (11) we employed the hierarchy in order to separate three-point expectation values,

$$\left\langle \hat{P}_{\mu}^{n,n}(t)\hat{b}_{\kappa}(t)\hat{P}_{\nu}^{m+1,m}(t')\right\rangle = p_{n}(t)\left\langle \hat{b}_{\kappa}(t)\hat{P}_{\nu}^{m+1,m}(t')\right\rangle^{\operatorname{corr}} + \mathcal{O}(1/Z^{2}).$$
 (12)

Here we restrict our considerations to order $\mathcal{O}(1/Z)$ which captures the free quasiparticle dynamics [42].

In general, depending on the particular observable, higher-order correlations must also be included. For example, particle-number correlations require three-point correlations as source terms and are therefore of order $\mathcal{O}(1/Z^2)$ [38, 58].

4. Double-time expectation values in equilibrium

The hierarchical set of equations for two-time expectation values induces a hierarchy for double-time Green's functions. This can be used for the computation of equilibrium correlation functions in the Bose–Hubbard model at finite temperatures. A thermal expectation value of an operator \hat{O} is defined as

$$\langle \hat{O} \rangle_{\rm th} = \frac{\operatorname{tr}(\hat{O}e^{-\beta\hat{H}})}{\operatorname{tr}(e^{-\beta\hat{H}})},\tag{13}$$

where $\beta = 1/k_b T$ is the inverse temperature. The retarded Green's function for the operators $\hat{A}_{\mu}(t)$ and $\hat{B}_{\nu}(t')$ is given by

$$G_{A_{\mu},B_{\nu}}(t,t') = \langle \langle \hat{A}_{\mu}(t); \hat{B}_{\nu}(t') \rangle \rangle = -i\Theta(t-t') \langle [\hat{A}_{\mu}(t), \hat{B}_{\nu}(t')] \rangle_{\rm th}, \qquad (14)$$

where we use the double brackets notation $\langle \langle \dots; \dots \rangle \rangle$ [60]. An analogous equation holds for the advanced Green's function. We choose $\hat{A}_{\mu} = \hat{P}_{\mu}^{n,n+1}$ and $\hat{B}_{\mu} = \hat{P}_{\mu}^{m+1,m}$ and find from equations (10) and (14) the relation

$$(i\partial_t - Un + \mu_0) \left\langle \left\langle \hat{P}^{n,n+1}_{\mu}(t); \hat{P}^{m+1,m}_{\mu}(t') \right\rangle \right\rangle = \delta(t) \delta_{m,n}(p_n - p_{n+1}).$$
(15)

An analogous equation of motion for the two-site Green functions can be deduced from (11). Via the Fourier transforms

$$\langle\langle\hat{P}^{n,n+1}_{\mu}(t);\hat{P}^{m+1,m}_{\mu}(t')\rangle\rangle = \int_{-\infty}^{\infty} d\omega \ e^{i\omega(t-t')}\langle\langle\hat{P}^{n,n+1};\hat{P}^{m+1,m}\rangle\rangle_{\omega}$$
(16)

and

$$\langle\langle \hat{P}^{n,n+1}_{\mu}(t); \hat{P}^{m+1,m}_{\nu}(t')\rangle\rangle^{\text{corr}} = \int_{-\infty}^{\infty} d\omega \ e^{i\omega(t-t')} \frac{1}{N} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot(\mathbf{x}_{\mu}-\mathbf{x}_{\nu})} \langle\langle \hat{P}^{n,n+1}; \hat{P}^{m+1,m}\rangle\rangle^{\text{corr}}_{\mathbf{k},\omega}$$
(17)

we can cast the differential equations for the Green functions into a set of algebraic equations,

$$(\omega - Un + \mu_0) \langle \langle \hat{P}^{n,n+1}; \hat{P}^{m+1,m} \rangle \rangle_\omega = \frac{\delta_{m,n}}{2\pi} (p_n - p_{n+1}), \qquad (18)$$

$$(\omega - Un + \mu_0) \langle \langle \hat{P}^{n,n+1}; \hat{P}^{m+1,m} \rangle \rangle_{\mathbf{k},\omega}^{\mathrm{corr}} = -JT_{\mathbf{k}} \sqrt{n+1} (p_n - p_{n+1}) \left[\langle \langle \hat{b}; \hat{P}^{m+1,m} \rangle \rangle_{\mathbf{k},\omega}^{\mathrm{corr}} - \langle \langle \hat{b}; \hat{P}^{m+1,m} \rangle \rangle_{\omega} \right].$$
(19)

Note that the Fourier transform w.r.t. time is possible as the on-site probabilities in thermal equilibrium p_n are time-independent. Beside the three-point correlation functions, we also neglected the back-reaction of two-site correlations onto the site-local Green function. Using the spectral decomposition of operators, thermal double-time correlation functions can be related to Green's functions [60] via

$$\langle \hat{B}(t)\hat{A}(t')\rangle_{\rm th} = i\lim_{\epsilon \to 0^+} \int_{-\infty}^{\infty} d\omega \frac{e^{i\omega(t-t')}}{e^{\beta\omega} - 1} \left[\langle \langle \hat{A}; \hat{B} \rangle \rangle_{\omega+i\epsilon} - \langle \langle \hat{A}; \hat{B} \rangle \rangle_{\omega-i\epsilon} \right]. \tag{20}$$

From equations (18) and (20) we obtain the on-site probabilities for n bosons on a lattice site in the absence of hopping,

$$p_n = \frac{e^{-\beta \left(\frac{U}{2}n(n-1)-\mu_0 n\right)}}{\sum_{m=0}^{\infty} e^{-\beta \left(\frac{U}{2}m(m-1)-\mu_0 m\right)}}.$$
(21)

The relation (19) determines the thermal expectation value of two-site correlation functions. For the particular case of a hyper-cubic lattice in D dimensions, we find a closed expression for the two-site correlation functions in terms of modified Bessel functions $I_{\alpha}(z)$,

$$\langle \hat{b}^{\dagger}_{\mu}(t)\hat{b}_{\nu}(t')\rangle_{\rm th}^{\rm corr} = -\frac{1}{\pi} \int d\omega \,\mathcal{P}\frac{1}{e^{\beta\omega} - 1} \int_{0}^{\infty} ds e^{-s + i\omega(t - t')} \\ \times \operatorname{Im} \left[G(\omega + i\epsilon) \prod_{j=1}^{D} (-1)^{\bigtriangleup \mathbf{x}^{j}_{\mu\nu}} I_{\bigtriangleup \mathbf{x}^{j}_{\mu\nu}} \left(\frac{JG(\omega + i\epsilon)s}{D} \right) \right], \quad (22)$$





Figure 1. Time-dependence of the two-time correlation functions $|\langle \hat{b}^{\dagger}_{\mu}(t) \hat{b}_{\mu}(t') \rangle_{\text{th}}^{\text{corr}}|^2$ as function of $t_{-} = (t - t')/2$ along the diagonal for a lattice in two dimensions for unit filling and J/U = 0.1. The parameters are (a) $\beta U = 1$, (b) $\beta U = 3$, (c) $\beta U = 5$, (d) $\beta U = \infty$. The red lines indicate the effective light cones which are determined from the low-temperature approximation of the maximum group velocity v_{max} . We see that v_{max} as well as the amplitude of the correlations decreases with the temperature of the thermal ensemble.

where $\Delta \mathbf{x}_{\mu\nu}^{j} = x_{\mu}^{j} - x_{\nu}^{j}$ is the *j*-component of the distance between two lattice sites and the spectral properties are determined by

$$G(\omega) = \sum_{n=0}^{\infty} \frac{(n+1)(p_n - p_{n+1})}{\omega - Un + \mu_0}.$$
(23)

The result for the correlation function (22) can be improved self-consistently via the inclusion of back-reaction terms or correlation functions of order $\mathcal{O}(1/Z^2)$. However, the corresponding algebraic equations can then only be solved numerically.

In figure 1 we depict double-time correlation functions for different values of βU . The density plots show a temperature-dependent light-cone structure [61–64]. For low temperatures it is viable to neglect occupation numbers n > 2. The dynamics of the correlation functions w.r.t. to the time difference $t_{-} = (t - t')/2$ at unit filling is determined by the frequencies

$$\Omega_{\mathbf{k}} = U - J(1 - 3p_0)T_{\mathbf{k}} - \sqrt{U^2 - 6J(1 - 3p_0)UT_{\mathbf{k}} + J^2(1 - 3p_0)^2T_{\mathbf{k}}^2}$$
(24)





Figure 2. Double-time correlation for $|x_{\mu} - x_{\nu}| = \sqrt{2}$ in two dimensions at different temperatures. The position of the maximum is shifting with temperature approximately as $(t_{-}J) \sim 1/(1-3p_0)$.

with $p_0 = p_2 = 1/(2 + e^{\beta U/2})$ being the probability to find zero or two particles on a lattice site. The maximum group velocity, given by $v^{\max} = \max_{\mathbf{k}} |\nabla_{\mathbf{k}} \Omega_{\mathbf{k}}|$, determines the light-cone structure of the correlations which is indicated by the red lines. At zero temperature, see figure 1(d), the propagation velocity of the correlations is maximal. In this limit, only the doublon-holon excitations $\langle P_{\mu}^{10}(t)P_{\nu}^{12}(t')\rangle^{\text{corr}}$, $\langle P_{\mu}^{21}(t)P_{\nu}^{01}(t')\rangle^{\text{corr}}$, and $\langle P_{\mu}^{21}(t)P_{\nu}^{12}(t')\rangle^{\text{corr}}$ are relevant. For finite temperatures, we have $1 - 3p_0 < 1$. According to equation (24), this implies a shrinking propagation velocity, see figure 1(c). If the temperature is increased even further, the approximation of thermal particle-hole excitations is not valid anymore since also occupation numbers n > 2 become relevant. In this case the analytical result (24) determines the light-cone structure rather poorly, see figures 1(a) and (b).

The population of higher excited states is also reflected in the time-evolution of the correlations at a fixed distance $|x_{\mu} - x_{\nu}|$. At $\beta U = \infty$, only eigen-modes of order $\mathcal{O}(U)$ play a role whereas for large temperatures the eigen-modes of order $\mathcal{O}(nU)$, n > 1 dominate the time-evolution, see figure 2.

5. Equilibration after a quantum quench

The time-evolution in the limit of zero temperature was discussed previously in [37, 38]. Here we turn to the non-equilibrium dynamics of excitations in the Bose–Hubbard system after a quantum quench at finite temperatures from J = 0 to J > 0. The evolution of time-local quantities can be deduced from double-time hierarchy for t = t' which coincides with single-time hierarchy in [37]. For large times, the correlation functions approach quasi-static values which differ from the corresponding thermal expectation values.

We assume the system to be initially in a thermal state where all sites are decoupled from each other and the occupation probability is determined by the thermal distribution p_n , see (21). The hopping rate is switched suddenly from J = 0 to a finite value which is still in the Mott regime $J < J_{\text{crit}}$. To zeroth order, the onsite-probabilities are not altered by the time evolution whereas in first order $\mathcal{O}(1/Z)$, the backreaction of the two-site correlations induces a non-trivial dynamics,

$$i\partial_t \langle \hat{P}^{n,n}_{\mu} \rangle = -\frac{J}{Z} \sum_{\kappa} T_{\mu\kappa} \bigg[\sqrt{n} \big(\langle \hat{P}^{n,n-1}_{\mu} \hat{b}_{\kappa} \rangle^{\text{corr}} - \langle \hat{b}^{\dagger}_{\kappa} \hat{P}^{n-1,n}_{\mu} \rangle^{\text{corr}} \big) \\ -\sqrt{n+1} \big(\langle \hat{P}^{n+1,n}_{\mu} \hat{b}_{\kappa} \rangle^{\text{corr}} - \langle \hat{b}^{\dagger}_{\kappa} \hat{P}^{n,n+1}_{\mu} \rangle^{\text{corr}} \big) \bigg].$$

$$(25)$$

The two-point correlations evolve according to

$$\begin{split} [i\partial_t + U(n-m)] \langle \hat{P}^{n+1,n}_{\mu} \hat{P}^{m,m+1}_{\nu} \rangle^{\text{corr}} \\ &= -\frac{J}{Z} \sqrt{n+1} (\langle \hat{P}^{n+1,n+1}_{\mu} \rangle - \langle \hat{P}^{n,n}_{\mu} \rangle) \sum_{\kappa \neq \mu,\nu} T_{\kappa\mu} \langle \hat{b}^{\dagger}_{\kappa} \hat{P}^{m,m+1}_{\nu} \rangle^{\text{corr}} \\ &- \frac{J}{Z} \sqrt{m+1} (\langle \hat{P}^{m,m}_{\nu} \rangle - \langle \hat{P}^{m+1,m+1}_{\nu} \rangle) \sum_{\kappa \neq \mu,\nu} T_{\kappa\nu} \langle \hat{P}^{n+1,n}_{\mu} \hat{b}_{\kappa} \rangle^{\text{corr}} \\ &- \frac{J}{Z} T_{\mu\nu} \sqrt{n+1} \sqrt{m+1} (\langle \hat{P}^{n+1,n+1}_{\mu} \rangle \langle \hat{P}^{m,m}_{\nu} \rangle - \langle \hat{P}^{n,n}_{\mu} \rangle \langle \hat{P}^{m+1,m+1}_{\nu} \rangle). \end{split}$$
(26)

For translational invariant initial conditions, equations (25) and (26) can be expressed in Fourier space. The lattice momentum **k** enters the equations (25) and (26) after the Fourier transform via $J_{\mathbf{k}} = \sum_{\mu} J_{\mu\nu} e^{i\mathbf{k}\cdot(\mathbf{x}_{\mu}-\mathbf{x}_{\nu})}/Z$. For a suitable initial state we can therefore assume that the Fourier components of the correlation functions $f_{\mathbf{k}}^{n,m} = \sum_{\mu} \langle \hat{P}_{\mu}^{n,n-1} \hat{P}_{\nu}^{m-1,m} \rangle e^{i\mathbf{k}\cdot(\mathbf{x}_{\mu}-\mathbf{x}_{\nu})}$ depend only on $J_{\mathbf{k}}$ via $f_{\mathbf{k}}^{n,m} \equiv f^{n,m}(J_{\mathbf{k}})$. The dynamics of the correlation functions in d dimensions is then governed by the nonlinear equations

$$i\partial_t P_n = -\int_{-J}^{J} d\Omega \,\rho_d(\Omega) \Omega \sum_m \sqrt{m+1} \bigg[\sqrt{n} \big(f^{n,m+1}(\Omega) - f^{m+1,n}(\Omega) \big) \\ -\sqrt{n+1} \big(f^{n+1,m+1}(\Omega) - f^{m+1,n+1}(\Omega) \big) \bigg]$$
(27)

and

$$[i\partial_t + U(n-m)]f^{n+1,m+1}(\Omega)$$

= $-\Omega \sum_{l=0}^{\infty} \sqrt{l+1} \left[\sqrt{n+1}(P_{n+1} - P_n)f^{l+1,m+1}(\Omega) + \sqrt{m+1}(P_m - P_{m+1})f^{n+1,l+1}(\Omega) \right]$

$$+ \int_{-J}^{J} d\Omega' \rho_{d}(\Omega') \Omega' \sum_{l=0}^{\infty} \sqrt{l+1} \bigg[\sqrt{n+1} (P_{n+1} - P_{n}) f^{l+1,m+1}(\Omega') \\ + \sqrt{m+1} (P_{m} - P_{m+1}) f^{n+1,l+1}(\Omega') \bigg] \\ - \Omega \sqrt{m+1} \sqrt{n+1} (P_{n+1} P_{m} - P_{n} P_{m+1}).$$
(28)

We introduced here the spectral density for a hypercubic lattice in d dimensions which can be represented as Fourier transform of Bessel functions,

$$\rho_d(\Omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} ds \, e^{is\omega} \left[\mathcal{J}_0\left(\frac{Js}{d}\right) \right]^d. \tag{29}$$

In figure 3 we show the time-evolution in two and three dimensions for various temperatures. The on-site probabilities are oscillating around their initial thermal value $P_n(t=0) = p_n$. The magnitude of the oscillations decreases with increasing temperature. Similarly, the magnitude of the next-neighbor correlation adopt their maximum value at zero temperature.

For sufficiently low temperatures, approximate analytical solutions of equations (27) and (28) can be found when the coupling between the different modes is neglected. As $\beta U \gg 1$, we can disregard occupations numbers greater than 2 and linearize (28) by replacing $P_n \to p_n$. At unit filling this implies the particle-hole symmetry $p_0 = p_2$. When the system is quenched from the initial state, the oscillations decay in time and the on-site probabilities approach for $t \to \infty$

$$P_{0/2,\text{equil}} = p_0 + \frac{1}{N} \sum_{\mathbf{k}} \frac{4J^2 T_{\mathbf{k}}^2 (1 - 4p_0 + 3p_0^2)}{\omega_{\mathbf{k}}^2}$$
(30)

with

$$\omega_{\mathbf{k}} = \sqrt{\left[U^2 - 6JT_{\mathbf{k}}(1 - 3p_0)U + J^2T_{\mathbf{k}}^2(1 - 3p_0)^2\right]}.$$
(31)

For the lattice-site correlations we obtain at large times the asymptotic expression

$$\langle \hat{b}_{\mu}^{\dagger} \hat{b}_{\nu} \rangle_{\text{equil}} = \frac{1}{N} \sum_{\mathbf{k}} e^{i\mathbf{k} \cdot (\mathbf{x}_{\mu} - \mathbf{x}_{\nu})} \frac{4JT_{\mathbf{k}}U(1 - 4p_0 + 3p_0^2)}{\omega_{\mathbf{k}}^2}.$$
(32)

Equations (30) and (32) confirm our statement that the quench-induced change of on-site probabilities and correlation functions diminishes with increasing temperature. As before we estimate the maximum propagation velocity from $v^{\max} = \max_{\mathbf{k}} |\nabla_{\mathbf{k}} \omega_{\mathbf{k}}|$. In a hyper-cubic lattice in D dimensions with small J/U we have $v^{\max} = J(3 - 9p_0)/D$ along the lattice axes and $v^{\max} = J(3 - 9p_0)/\sqrt{D}$ along the diagonals, see figure 4.

We can compare the pre-thermalized state with a corresponding thermal state that has the same temperature T and filling $\langle \hat{n}_{\mu} \rangle$. The asymptotic values of the on-site probabilities $P_{n,\text{equil}}$ and the correlation functions $\langle \hat{b}_{\mu}^{\dagger} \hat{b}_{\nu} \rangle_{\text{equil}}$ are deduced from equations (27)





Figure 3. Equilibration dynamics of the Bose–Hubbard system in two and three dimensions at unit filling. In the bottom row, we have shown the correlations between the nearest neighbor sites μ and ν . The system is quenched from a thermal state at J = 0 to J/U = 0.1. In our computation, we did not restrict the occupation number. Nevertheless, we see that also for finite but sufficiently low temperatures, the particle-hole symmetry $P_0 = P_2$ is approximately valid.

and (28). The thermal correlation $\langle \hat{b}^{\dagger}_{\mu} \hat{b}_{\nu} \rangle_{\text{th}}$ can be computed from equation (22). For the order $\mathcal{O}(1/Z)$ -contribution of the $P_{n,\text{therm}}$ we refer to an earlier publication [41]. Explicitly we have (see equation (21) in [41])





Figure 4. Maximum propagation velocity of the correlations as function of the temperature of the initial ensemble.

$$P_{n,\text{therm}} = p_n + \frac{1}{N} \sum_{\mathbf{k}} \sum_{l=-\infty}^{\infty} \frac{JT_{\mathbf{k}}}{1 + JT_{\mathbf{k}}G(\omega_l)} \left[p_n G(\omega_l) - \frac{(n+1)p_n}{\omega_l - Un + \mu} + \frac{np_n}{\omega_l - U(n-1) + \mu} + \frac{n(p_{n-1} - p_n)}{\beta(\omega_l - U(n-1) + \mu)^2)^2} - \frac{(n+1)(p_n - p_{n+1})}{\beta(\omega_l - Un + \mu)^2} \right]$$
(33)

with the bosonic Matsubara modes $\omega_l = 2\pi i l/\beta$.

At zero temperature, the prethermalized and the thermal value for the P_0 and P_2 differ roughly by a factor of 2 which has been stated elsewhere [65]. For sufficiently low temperatures, the particle-hole symmetry is valid, $P_0 \sim P_2$, which can be deduced from comparing figures 5(a) and (b) or figures 5(d) and (e). The energy which is transferred by a quench to the system becomes more and more irrelevant for increasing temperatures. Thus, the difference between thermal and pre-thermalized quantities reduces with growing *T*. From figures 5(c) and (f) we see how the increasing temperature diminishes the correlations between lattice sites. However, the thermal next neighbor correlation function has its global maximum at finite T > 0.

Within our first-order (in 1/Z) approach, we obtain the first stage of relaxation which is also known as pre-thermalization, see, e.g. [38, 39, 43, 66–68]. This can be understood as dephasing of the quasi-particle excitations and does not imply a real thermalization process. True equilibration sets in on larger time scales and requires higher-order correlation functions. In [43–46] we show that the thermalization process can be described by taking into account correlations which are of third order in 1/Z. Their time-evolution then leads to an effective Boltzmann equation which describes the approach of the quasi-particle distribution functions to their thermal distribution via two-body collisions.



Figure 5. After a quantum quench at a temperature T, the occupation probabilities and the correlation functions approach a prethermalized value (red curves). This is compared with the corresponding thermal expressions (black curves). For low temperatures, the onsite-quantities differ roughly by a factor of 2. The difference between prethermalized and thermal values diminishes with increasing temperatures. Note that deviations from the particle-hole symmetry at high temperatures are larger in three dimensions (see (d) and (e)) than in two dimensions (see (a) and (b)). In (c) and (f) we depict the temperature-dependence of the prethermalized and thermal expectation values of the next neighbor correlations $\langle \hat{b}^{\dagger}_{\mu} \hat{b}_{\nu} \rangle$. The thermal correlation function has its global maximum at a finite temperature.

6. Quantum quench and double-time correlations

A quantum quench changes also the light-cone structure of the double-time correlation functions. For simplicity, we restrict our considerations to zero temperature and assume that the system is initially in an equilibrium state with a finite hopping rate J_- . At time t=0, the hopping rate is quenched to a value $J_+ < J_{crit}$. Here the Fourier components of the correlation functions depend on two times

$$\langle \hat{P}^{n,n-1}_{\mu}(t)\hat{P}^{m-1,m}_{\nu}(t')\rangle^{\rm corr} = \frac{1}{N}\sum_{\bf k} f^{n,m}_{\bf k}(t,t')e^{i{\bf k}\cdot({\bf x}_{\mu}-{\bf x}_{\nu})}.$$
 (34)

The dynamics of the correlation functions follows directly from equation (11). Neglecting the back-reaction onto the on-site probabilities, the Fourier coefficients evolve up to order 1/Z according to

$$i\partial_t f_{\mathbf{k}}^{11} = -J_{\pm} T_{\mathbf{k}} (f_{\mathbf{k}}^{11} + \sqrt{2} f_{\mathbf{k}}^{21}) - J_{\pm} T_{\mathbf{k}}, \qquad (35)$$

$$i\partial_t f_{\mathbf{k}}^{12} = -J_{\pm} T_{\mathbf{k}} (f_{\mathbf{k}}^{12} + \sqrt{2} f_{\mathbf{k}}^{22}), \qquad (36)$$

$$i\partial_t f_{\mathbf{k}}^{21} = \sqrt{2}J_{\pm}T_{\mathbf{k}}(f_{\mathbf{k}}^{11} + \sqrt{2}f_{\mathbf{k}}^{21}) - Uf_{\mathbf{k}}^{21} + \sqrt{2}J_{\pm}T_{\mathbf{k}}, \qquad (37)$$

$$i\partial_t f_{\mathbf{k}}^{22} = \sqrt{2}J_{\pm}T_{\mathbf{k}}(f_{\mathbf{k}}^{12} + \sqrt{2}f_{\mathbf{k}}^{22}) - Uf_{\mathbf{k}}^{22}.$$
(38)

Similarly, we find the time-evolution w.r.t. variable t'

$$i\partial_{t'}f_{\mathbf{k}}^{11} = J_{\pm}T_{\mathbf{k}}(f_{\mathbf{k}}^{11} + \sqrt{2}f_{\mathbf{k}}^{12}) + J_{\pm}T_{\mathbf{k}}, \qquad (39)$$

$$i\partial_{t'}f_{\mathbf{k}}^{12} = -\sqrt{2}J_{\pm}T_{\mathbf{k}}(f_{\mathbf{k}}^{11} + \sqrt{2}f_{\mathbf{k}}^{12}) + Uf_{\mathbf{k}}^{12} - \sqrt{2}J_{\pm}T_{\mathbf{k}}, \qquad (40)$$

$$i\partial_{t'}f_{\mathbf{k}}^{21} = J_{\pm}T_{\mathbf{k}}(f_{\mathbf{k}}^{21} + \sqrt{2}f_{\mathbf{k}}^{22}), \qquad (41)$$

$$i\partial_{t'}f_{\mathbf{k}}^{22} = -\sqrt{2}J_{\pm}T_{\mathbf{k}}(f_{\mathbf{k}}^{21} + \sqrt{2}f_{\mathbf{k}}^{22}) + Uf_{\mathbf{k}}^{22}.$$
(42)

For t, t' < 0, the correlation functions can be immediately obtained from the ground state correlations at $J = J_{-}$ [38]. Due to the quantum quench, the correlation function is not anymore homogeneous in time but depends on the relative time $t_{-} = (t - t')/2$ and on the central time $t_{+} = (t + t')/2$. For $t_{+} \pm t_{-} < 0$ and $t_{+} \pm t_{-} > 0$ we find correlations before and after the hopping quench, respectively. Correlations between the annihilation (creation) of a particle before the quench and the creation (annihilation) of particle after the quench can be obtained for $t_{+} + t_{-} > 0$ and $t_{+} - t_{-} < 0$ ($t_{+} + t_{-} > 0$ and $t_{+} - t_{-} < 0$).





Figure 6. Double-time correlation function $\langle \hat{b}^{\dagger}_{\mu}(t)\hat{b}_{\nu}(t')\rangle_{T=0}$ in one dimension for a quench at t = 0 from $J_{-}/U = 0.05$ to $J_{+}/U = 0.15$. (a): $t_{+}U = 100$, the lightcone has a kink at $t_{-} = t_{+}$ where the maximum velocity changes from $v_{++}^{\max} \approx 0.40$ to $v_{+-}^{\max} \approx 0.24$. (b): $t_{+}U = -100$, the lightcone has a kink at $t_{-} = -t_{+}$ where the maximum velocity changes from $v_{--}^{\max} \approx 0.10$ to $v_{+-}^{\max} \approx 0.24$.

The light-cone structure is primarily determined by three different velocities. For t, t' < 0, the maximum velocity $v_{--}^{\max} = \max_{\mathbf{k}} |\nabla_{\mathbf{k}} \Omega_{\mathbf{k}}^{--}|$ can be estimated from

$$\Omega_{\mathbf{k}}^{--} = U - J_{-}T_{\mathbf{k}} - \sqrt{U^{2} - 6J_{-}UT_{\mathbf{k}} + (J_{-}T_{\mathbf{k}})^{2}}.$$
(43)

For t > 0 and t' < 0 or t < 0 and t' > 0, the spread is determined by both hopping rates J_{-} and J_{+} . Thus we have the eigen-modes

$$\Omega_{\mathbf{k}}^{+-} = \frac{1}{2} \left(U - J_{-}T_{\mathbf{k}} - \sqrt{U^{2} - 6J_{-}UT_{\mathbf{k}} + (J_{-}T_{\mathbf{k}})^{2}} \right) + \frac{1}{2} \left(U - J_{+}T_{\mathbf{k}} - \sqrt{U^{2} - 6J_{+}UT_{\mathbf{k}} + (J_{+}T_{\mathbf{k}})^{2}} \right).$$
(44)

from which one can obtain $v_{+-}^{\max} = \max_{\mathbf{k}} |\nabla_{\mathbf{k}} \Omega_{\mathbf{k}}^{+-}|$. Finally, if t, t' > 0, the spread of correlations is dominantly determined by J_+ . Here the maximum velocity $v_{++}^{\max} = \max_{\mathbf{k}} |\nabla_{\mathbf{k}} \Omega_{\mathbf{k}}^{++}|$ can be derived from

$$\Omega_{\mathbf{k}}^{++} = U - J_{+}T_{\mathbf{k}} - \sqrt{U^{2} - 6J_{+}UT_{\mathbf{k}} + (J_{+}T_{\mathbf{k}})^{2}}.$$
(45)

The kink in the light-cone structure due to the quantum quench is illustrated in figure 6.

7. Conclusions

We studied equilibrium properties and non-equilibrium dynamics of the Bose–Hubbard model in the Mott insulating phase. To this end, we extended the hierarchy for large coordination numbers Z presented in [37] to a hierarchy for double-time correlation functions.

This enabled us to derive thermal correlation functions and we studied the spread of two-time correlation functions at finite initial temperatures, see figures 1 and 2. We restricted our considerations to first order in 1/Z which governs the free quasi-particle evolution. As usual, the effective light-cone structure was obtained via a saddle-point approximation.

As we demonstrated above, the dynamics of strongly interacting quantum manybody systems and their thermal properties can be both accessed within our approach. The phenomenon of pre-thermalization after a quantum quench was generalized from T = 0 [38] to finite temperatures, see figures 3 and 4. Note that the dynamical equations in order $\mathcal{O}(1/Z)$ cover only the short-time evolution of the excitations. In order to include the long-time evolution which is determined by quasi-particle scattering, also higher order correlations have to be taken into account. For real thermalization processes, for example, one has to evaluate the hierarichal equations up to order $\mathcal{O}(1/Z^3)$ in order to obtain a Boltzmann equation [43, 44].

Apart from these theoretical investigations, our approach can also be applied in order to interpret experimental results. Since the double-time hierarchy induces a Green function hierarchy, the latter can used for the interpretation of pump-probe experiments [69]. An excitation which is created by a pump beam at time t and measured by a probe beam at time t' is naturally described in terms of the lesser Green functions [10, 69, 70]. Moreover, the Green function hierarchy allows for a controlled perturbative calculation of the self-energy or the susceptibility of strongly correlated systems.

As an outlook, the study of out-of-time-correlators, a common measure for quantum chaos, should be feasible within our approach [71, 72]. In this context one has to extend the double-time hierarchy of correlations to a hierarchy of multi-time correlations. This should be possible in complete analogy to the approach presented in this work and will be the subject of further studies.

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Appendix. Proof of the hierarchy

The most general double-time expectation value has the form $\langle \hat{A}_{\mathcal{S}}(t)\hat{B}_{\mathcal{S}}(t')\rangle$ where \mathcal{S} denotes the set of $|\mathcal{S}|$ lattice sites. In order to avoid cluttering of indices, we introduce a short hand notation for operators which are defined on the set \mathcal{S} via $\hat{A}_{\mathcal{S}}(t) = \hat{A}_{\mu_1}^1(t) \times \ldots \times \hat{A}_{\mu_n}^n(t)$ and $\hat{B}_{\mathcal{S}}(t') = \hat{B}_{\mu_1}^1(t') \times \ldots \times \hat{B}_{\mu_n}^n(t')$. From the equation-of-motion hierarchy for the expectation values $\langle \hat{A}_{\mathcal{S}}(t)\hat{B}_{\mathcal{S}}(t') \rangle$, the hierarchy for expectation values of the form $\langle \hat{A}(t)_{\mathcal{P}_1}\hat{B}_{\mathcal{P}_2}(t') \rangle$ can be obtained by setting $\mathcal{S} = \mathcal{P}_1 \cup \mathcal{P}_2$ and choosing $\hat{A}_{\mu}(t) = \hat{1}_{\mu}$ for $\mu \notin \mathcal{P}_1$ and $\hat{B}_{\nu}(t') = \hat{1}_{\nu}$ for $\nu \notin \mathcal{P}_2$.

In [37], we presented a hierarchy for the correlated parts of a many-particle density matrix based on a large coordination number Z. This hierarchy was formulated for operators but it can also be stated in terms of correlation functions. In the following, we will derive the corresponding hierarchy for two-time correlation functions. The starting point is a separation of the correlation functions in correlated and uncorrelated parts. For better readability, we make the replacement $\langle \ldots \rangle^{\text{corr}} \rightarrow \langle \ldots \rangle^{\text{c}}$ in our notation. General correlation functions can be separated according to

$$\langle \hat{A}_{\mathcal{S}}(t)\hat{B}_{\mathcal{S}}(t')\rangle^{c} = \langle \hat{A}_{\mathcal{S}}(t)\hat{B}_{\mathcal{S}}(t')\rangle - \sum_{\bigcup_{i}\mathcal{P}_{i}=\mathcal{S},\mathcal{P}_{i}\subset\mathcal{S}}\prod_{\mathcal{P}_{i}}\langle \hat{A}_{\mathcal{P}_{i}}(t)\hat{B}_{\mathcal{P}_{i}}(t')\rangle^{c},$$
(A.1)

where the sum is over all proper partitions of the set S. Note that the definition of the correlated parts agrees with the separation of the density matrix into correlated parts given in [37] if the operators depending on t (or t') are replaced by the unit operator. As in [37] we assume that the hierarchy of correlations is valid at some time t_0 . For the Bose–Hubbard system, this can be achieved by choosing initially a factorizing Mott insulator state for J=0. The hopping rate J can then be changed to a finite value in the insulator phase. Due to the finite Mott gap, the quantum state stays close to the ground state during this adiabatic switching procedure. Thus, the hierarchy of correlations is satisfied initially and remains valid during the subsequent (quench) dynamics, see below. An analogous argument can be applied to thermal states, as long as we are in the Mott insulating phase. Since a thermal state is an incoherent superposition of eigenstates, one can start with a suitable incoherent superposition (ensemble) of factorizing eigenstates at J=0, which transform into the desired thermal ensemble after switching J adiabatically.

The central point of our derivation is the scaling hierarchy of the correlations,

$$\langle \hat{A}_{\mathcal{S}}(t)\hat{B}_{\mathcal{S}}(t')\rangle^{c} = \mathcal{O}(Z^{1-|\mathcal{S}|}).$$
(A.2)

Rewriting the hierarchy of the density matrix from [37] in terms of expectation values it is possible to guess the corresponding hierarchy for for the equations of motion of $\langle \hat{A}_{\mathcal{S}}(t)\hat{B}_{\mathcal{S}}(t')\rangle^{c}$. We claim that for a lattice Hamiltonian of the form

$$\hat{H} = -\frac{J}{Z} \sum_{\mu,\nu} T_{\mu\nu} \hat{X}^{\dagger}_{\mu} \hat{X}_{\nu} + \sum_{\mu} \hat{H}_{\mu}, \qquad (A.3)$$

the full hierarchy of correlations reads

$$i\partial_t \langle \hat{A}_{\mathcal{S}}(t)\hat{B}_{\mathcal{S}}(t')\rangle^{c} = \sum_{\mu\in\mathcal{S}} \langle [\hat{A}_{\mathcal{S}}(t), \hat{H}_{\mu}(t)]\hat{B}_{\mathcal{S}}(t')\rangle^{c} - \frac{J}{Z} \sum_{\mu,\nu\in\mathcal{S}} T_{\mu\nu} \langle [\hat{A}_{\mathcal{S}}(t), \hat{X}^{\dagger}_{\mu}(t)\hat{X}_{\nu}(t)]\hat{B}_{\mathcal{S}}(t')\rangle^{c}$$
(A.4)

$$-\frac{J}{Z}\sum_{\kappa\notin\mathcal{S}}\sum_{\mu\in\mathcal{S}}T_{\mu\kappa}\left\{\langle\hat{X}^{\dagger}_{\kappa}(t)[\hat{A}_{\mathcal{S}}(t),\hat{X}_{\mu}(t)]\hat{B}_{\mathcal{S}}(t')\rangle^{c}+\langle\hat{X}_{\kappa}(t)[\hat{A}_{\mathcal{S}}(t),\hat{X}^{\dagger}_{\mu}(t)]\hat{B}_{\mathcal{S}}(t')\rangle^{c}\right\}$$
(A.5)

$$-\frac{J}{Z}\sum_{\kappa\notin\mathcal{S}}\sum_{\mu\in\mathcal{S}}\sum_{\mathcal{P}\subseteq\mathcal{S}\setminus\{\mu\}}^{\mathcal{P}\cup\bar{\mathcal{P}}=\mathcal{S}\setminus\{\mu\}}T_{\mu\kappa}\bigg\{\langle [\hat{A}_{\mathcal{P}\cup\{\mu\}}(t),\hat{X}_{\mu}(t)]\hat{B}_{\mathcal{P}\cup\{\mu\}}(t')\rangle^{c}\langle \hat{X}_{\kappa}^{\dagger}(t)\hat{A}_{\bar{\mathcal{P}}}(t)\hat{B}_{\bar{\mathcal{P}}}(t')\rangle^{c}$$
(A.6)

$$+\left\langle [\hat{A}_{\mathcal{P}\cup\{\mu\}}(t), \hat{X}^{\dagger}_{\mu}(t)]\hat{B}_{\mathcal{P}\cup\{\mu\}}(t')\right\rangle^{c}\left\langle \hat{X}_{\kappa}(t)\hat{A}_{\bar{\mathcal{P}}}(t)\hat{B}_{\bar{\mathcal{P}}}(t')\right\rangle^{c}\right\}$$
(A.7)

$$-\frac{J}{Z}\sum_{\mu,\nu\in\mathcal{S}}\sum_{\mathcal{P}\subseteq\mathcal{S}\backslash\{\mu,\nu\}}^{\mathcal{P}\cup\bar{\mathcal{P}}=\mathcal{S}\backslash\{\mu,\nu\}}T_{\mu\nu}\Bigg\{\langle [\hat{A}_{\mathcal{P}\cup\{\mu\}}(t),\hat{X}^{\dagger}_{\mu}(t)]\hat{B}_{\mathcal{P}\cup\{\mu\}}(t')\rangle^{c}\langle \hat{X}_{\nu}(t)\hat{A}_{\bar{\mathcal{P}}\cup\{\nu\}}(t)\hat{B}_{\bar{\mathcal{P}}\cup\{\nu\}}(t')\rangle^{c}$$
(A.8)

$$+ \langle \hat{A}_{\mathcal{P}\cup\{\mu\}}(t) \hat{X}^{\dagger}_{\mu}(t) \hat{B}_{\mathcal{P}\cup\{\mu\}}(t') \rangle^{c} \langle [\hat{A}_{\bar{\mathcal{P}}\cup\{\nu\}}(t), \hat{X}_{\nu}(t)] \hat{B}_{\bar{\mathcal{P}}\cup\{\nu\}}(t') \rangle^{c}$$
(A.9)

$$-\langle \hat{A}_{\mathcal{P}\cup\nu}(t)\hat{B}_{\mathcal{P}\cup\nu}(t')\rangle^{c} \times \left[\langle \hat{X}_{\nu}^{\dagger}(t)[\hat{A}_{\bar{\mathcal{P}}\cup\{\mu\}}(t),\hat{X}_{\mu}(t)]\hat{B}_{\bar{\mathcal{P}}\cup\{\mu\}}(t')\rangle^{c} + \langle \hat{X}_{\nu}(t)[\hat{A}_{\bar{\mathcal{P}}\cup\{\mu\}}(t),\hat{X}_{\mu}^{\dagger}(t)]\hat{B}_{\bar{\mathcal{P}}\cup\{\mu\}}(t')\rangle^{c}\right]$$

$$(A.10)$$

$$+\sum_{\mathcal{Q}\subseteq\bar{\mathcal{P}}}^{\mathcal{Q}\cup\bar{\mathcal{Q}}=\bar{\mathcal{P}}} \left(\langle [\hat{A}_{\mathcal{Q}\cup\{\mu\}}(t), \hat{X}_{\mu}(t)] \hat{B}_{\mathcal{Q}\cup\{\mu\}}(t') \rangle^{c} \langle \hat{X}_{\nu}^{\dagger}(t) \hat{A}_{\bar{\mathcal{Q}}}(t) \hat{B}_{\bar{\mathcal{Q}}}(t') \rangle^{c} \right)$$
(A.11)

$$+\left\langle [\hat{A}_{\mathcal{Q}\cup\{\mu\}}(t), \hat{X}^{\dagger}_{\mu}(t)] \hat{B}_{\mathcal{Q}\cup\{\mu\}}(t') \right\rangle^{c} \left\langle \hat{X}_{\nu}(t) \hat{A}_{\bar{\mathcal{Q}}}(t) \hat{B}_{\bar{\mathcal{Q}}}(t') \right\rangle^{c} \right\rangle \right\}.$$
(A.12)

Both sides of equations (A.4)–(A.12) have the same order in 1/Z. We will restrict ourselves to bosonic systems for proving (A.4)–(A.12) by induction. For fermionic operators, additional signs will appear due to the permutations of the operators \hat{A}_{μ} and \hat{B}_{μ} .

To begin, we assume that the hierarchy holds for all sets of lattice sites with cardinality *strictly less* then |S|. From this we will derive the equations of motion for a set with cardinality *equal* to |S|. The Heisenberg equations of motion for the operator \hat{A}_{S} lead to

$$i\partial_{t}\langle\hat{A}_{\mathcal{S}}(t)\hat{B}_{\mathcal{S}}(t')\rangle = \sum_{\mu\in\mathcal{S}}\langle[\hat{A}_{\mathcal{S}}(t),\hat{H}_{\mu}(t)]\hat{B}_{\mathcal{S}}(t')\rangle$$
$$-\frac{J}{Z}\sum_{\mu,\nu\in\mathcal{S}}T_{\mu\nu}\langle[\hat{A}_{\mathcal{S}}(t),\hat{X}_{\mu}^{\dagger}(t)\hat{X}_{\nu}(t)]\hat{B}_{\mathcal{S}}(t')\rangle$$
$$-\frac{J}{Z}\sum_{\kappa\notin\mathcal{S}}\sum_{\mu\in\mathcal{S}}T_{\mu\kappa}\langle\hat{X}_{\kappa}^{\dagger}(t)[\hat{A}_{\mathcal{S}}(t),\hat{X}_{\mu}(t)]\hat{B}_{\mathcal{S}}(t')\rangle$$
$$-\frac{J}{Z}\sum_{\kappa\notin\mathcal{S}}\sum_{\mu\in\mathcal{S}}T_{\mu\kappa}\langle\hat{X}_{\kappa}(t)[\hat{A}_{\mathcal{S}}(t),\hat{X}_{\mu}^{\dagger}(t)]\hat{B}_{\mathcal{S}}(t')\rangle.$$
(A.13)

As a next step, we separate the expectation values into correlated parts according to (A.1). The first term can be written as

$$(0) = \sum_{\mu \in \mathcal{S}} \langle [\hat{A}_{\mathcal{S}}(t), \hat{H}_{\mu}(t)] \hat{B}_{\mathcal{S}}(t') \rangle = \sum_{\mathcal{P} \subseteq \mathcal{S} \setminus \{\mu\}} \langle [\hat{A}_{\mathcal{P} \cup \{\mu\}}(t), \hat{H}_{\mu}(t)] \hat{B}_{\mathcal{P} \cup \{\mu\}}(t') \rangle$$
$$\times \sum_{\cup_{i} \mathcal{P}_{i} = \mathcal{S} \setminus \mathcal{P} \cup \{\mu\}} \prod_{\mathcal{P}_{i}} \langle \hat{A}_{\mathcal{P}_{i}}(t) \hat{B}_{\mathcal{P}_{i}}(t') \rangle^{c}.$$
(A.14)

The second term on the right hand side of equation (A.13) can be expanded as

$$-\frac{J}{Z}\sum_{\mu,\nu\in\mathcal{S}}T_{\mu\nu}\langle [\hat{A}_{\mathcal{S}}(t),\hat{X}^{\dagger}_{\mu}(t)\hat{X}_{\nu}(t)]\hat{B}_{\mathcal{S}}(t')\rangle = (1) + (2a) + (2b)$$
(A.15)

with

$$(1) = -\frac{J}{Z} \sum_{\mu,\nu\in\mathcal{S}} T_{\mu\nu} \sum_{\mathcal{P}\subseteq\mathcal{S}\setminus\{\mu,\nu\}} \langle [\hat{A}_{\mathcal{P}\cup\{\mu\nu\}}(t), \hat{X}_{\mu}(t)^{\dagger} \hat{X}_{\nu}(t)] \hat{B}_{\mathcal{P}\cup\{\mu\nu\}}(t') \rangle^{c} \\ \times \sum_{\cup_{i}\mathcal{P}_{i}=\mathcal{S}\setminus\mathcal{P}\cup\{\mu,\nu\}} \prod_{\mathcal{P}_{i}} \langle \hat{A}_{\mathcal{P}_{i}}(t) \hat{B}_{\mathcal{P}_{i}}(t') \rangle^{c}, \qquad (A.16)$$

$$(2a) - \frac{J}{Z} \sum_{\mu,\nu\in\mathcal{S}} T_{\mu\nu} \sum_{\mathcal{P}\subseteq\mathcal{S}\setminus\{\mu,\nu\}} \left(\sum_{\bigcup_{i}\mathcal{P}_{i}=\mathcal{S}\setminus\mathcal{P}\cup\{\mu,\nu\}} \prod_{\mathcal{P}_{i}} \langle \hat{A}_{\mathcal{P}_{i}}(t)\hat{B}_{\mathcal{P}_{i}}(t')\rangle^{c} \right) \\ \times \sum_{\mathcal{Q}\subseteq\mathcal{P}}^{\mathcal{Q}\cup\bar{\mathcal{Q}}=\mathcal{P}} \langle [\hat{A}_{\mathcal{Q}\cup\{\mu\}}(t),\hat{X}_{\mu}^{\dagger}(t)]\hat{B}_{\mathcal{Q}\cup\{\mu\}}(t')\rangle^{c} \langle \hat{X}_{\nu}(t)\hat{A}_{\bar{\mathcal{Q}}(t)\cup\{\nu\}}(t)\hat{B}_{\bar{\mathcal{Q}}\cup\{\nu\}}(t')\rangle^{c}, \quad (A.17)$$

and

$$(2b) = -\frac{J}{Z} \sum_{\mu,\nu\in\mathcal{S}} T_{\mu\nu} \sum_{\mathcal{P}\subseteq\mathcal{S}\backslash\{\mu,\nu\}} \left(\sum_{\bigcup_i \mathcal{P}_i = \mathcal{S}\backslash\mathcal{P}\cup\{\mu,\nu\}} \prod_{\mathcal{P}_i} \langle \hat{A}_{\mathcal{P}_i}(t)\hat{B}_{\mathcal{P}_i}(t') \rangle^{\mathsf{c}} \right) \\ \times \sum_{\mathcal{Q}\subseteq\mathcal{P}}^{\mathcal{Q}\cup\bar{\mathcal{Q}}=\mathcal{P}} \langle \hat{A}_{\mathcal{Q}\cup\{\mu\}}(t)\hat{X}^{\dagger}_{\mu}(t)\hat{B}_{\mathcal{Q}\cup\{\mu\}}(t') \rangle^{\mathsf{c}} \langle [\hat{A}_{\bar{\mathcal{Q}}\cup\{\nu\}}(t),\hat{X}_{\nu}(t)]\hat{B}_{\bar{\mathcal{Q}}\cup\{\nu\}}(t') \rangle^{\mathsf{c}}.$$
(A.18)

The third term on the right hand side of equation (A.13) can be written as

$$-\frac{J}{Z}\sum_{\kappa\notin\mathcal{S}}\sum_{\mu\in\mathcal{S}}T_{\mu\kappa}\langle\hat{X}^{\dagger}_{\kappa}(t)[\hat{A}_{\mathcal{S}}(t),\hat{X}_{\mu}(t)]\hat{B}_{\mathcal{S}}(t')\rangle = (3a) + (4a)$$
(A.19)

with

$$(3a) = -\frac{J}{Z} \sum_{\kappa \notin S} \sum_{\mu \in S} T_{\mu\kappa} \sum_{\mathcal{P} \subseteq \mathcal{S} \setminus \{\mu\}} \left(\sum_{\bigcup_i \mathcal{P}_i = \mathcal{S} \setminus \mathcal{P} \cup \{\mu\}} \prod_{\mathcal{P}_i} \langle \hat{A}_{\mathcal{P}_i}(t) \hat{B}_{\mathcal{P}_i}(t') \rangle^{c} \right) \\ \times \langle \hat{X}^{\dagger}_{\kappa}(t) [\hat{A}_{\mathcal{P} \cup \{\mu\}}(t), \hat{X}_{\mu}(t)] \hat{B}_{\mathcal{P} \cup \{\mu\}}(t') \rangle^{c}$$
(A.20)

and

$$(4a) = -\frac{J}{Z} \sum_{\kappa \notin S} \sum_{\mu \in S} T_{\mu\kappa} \sum_{\mathcal{P} \subseteq S \setminus \{\mu\}} \left(\sum_{\bigcup_i \mathcal{P}_i = S \setminus \mathcal{P} \cup \{\mu\}} \prod_{\mathcal{P}_i} \langle \hat{A}_{\mathcal{P}_i}(t) \hat{B}_{\mathcal{P}_i}(t') \rangle^{\mathsf{c}} \right) \\ \times \sum_{\mathcal{Q} \subseteq \mathcal{P}}^{\mathcal{Q} \cup \bar{\mathcal{Q}} = \mathcal{P}} \langle [\hat{A}_{\mathcal{Q} \cup \{\mu\}}(t), \hat{X}_{\mu}(t)] \hat{B}_{\mathcal{Q} \cup \{\mu\}}(t') \rangle^{\mathsf{c}} \langle \hat{X}_{\kappa}^{\dagger}(t) \hat{A}_{\bar{\mathcal{Q}}}(t) \hat{B}_{\bar{\mathcal{Q}}}(t') \rangle^{\mathsf{c}}. \quad (A.21)$$

Similarly, for the last summand in equation (A.13) we have

$$-\frac{J}{Z}\sum_{\kappa\notin\mathcal{S}}\sum_{\mu\in\mathcal{S}}T_{\mu\kappa}\langle\hat{X}_{\kappa}(t)[\hat{A}_{\mathcal{S}}(t),\hat{X}^{\dagger}_{\mu}(t)]\hat{B}_{\mathcal{S}}(t')\rangle = (3b) + (4b)$$
(A.22)

with

$$(3b) = -\frac{J}{Z} \sum_{\kappa \notin S} \sum_{\mu \in S} T_{\mu\kappa} \sum_{\mathcal{P} \subseteq S \setminus \{\mu\}} \left(\sum_{\bigcup_i \mathcal{P}_i = S \setminus \mathcal{P} \cup \{\mu\}} \prod_{\mathcal{P}_i} \langle \hat{A}_{\mathcal{P}_i}(t) \hat{B}_{\mathcal{P}_i}(t') \rangle^{c} \right) \\ \times \langle \hat{X}_{\kappa}(t) [\hat{A}_{\mathcal{P} \cup \{\mu\}}(t), \hat{X}^{\dagger}_{\mu}(t)] \hat{B}_{\mathcal{P} \cup \{\mu\}}(t') \rangle^{c}$$
(A.23)

and

$$(4b) = -\frac{J}{Z} \sum_{\kappa \notin S} \sum_{\mu \in S} T_{\mu\kappa} \sum_{\mathcal{P} \subseteq S \setminus \{\mu\}} \left(\sum_{\bigcup_i \mathcal{P}_i = S \setminus \mathcal{P} \cup \{\mu\}} \prod_{\mathcal{P}_i} \langle \hat{A}_{\mathcal{P}_i}(t) \hat{B}_{\mathcal{P}_i}(t') \rangle^{\mathrm{c}} \right) \\ \times \sum_{\mathcal{Q} \subseteq \mathcal{P}}^{\mathcal{Q} \cup \bar{\mathcal{Q}} = \mathcal{P}} \langle [\hat{A}_{\mathcal{Q} \cup \{\mu\}}(t), \hat{X}^{\dagger}_{\mu}(t)] \hat{B}_{\mathcal{Q} \cup \{\mu\}}(t') \rangle^{\mathrm{c}} \langle \hat{X}_{\kappa}(t) \hat{A}_{\bar{\mathcal{Q}}}(t) \hat{B}_{\bar{\mathcal{Q}}}(t') \rangle^{\mathrm{c}}.$$
(A.24)

We want to derive the equation of motion for the correlator $\langle \hat{A}_{\mathcal{S}}(t)\hat{B}_{\mathcal{S}}(t')\rangle^{c}$ which was defined in equation (A.1). The equation of motion for the first term on the right hand side of (A.1) is given by (A.14)–(A.24). The time derivative of the second term on the right hand side in equation (A.1) reads

$$i\partial_{t} \sum_{\bigcup_{i} \mathcal{P}_{i} = \mathcal{S}, \mathcal{P}_{i} \subset \mathcal{S}} \prod_{\mathcal{P}_{i}} \langle \hat{A}_{\mathcal{P}_{i}}(t) \hat{B}_{\mathcal{P}_{i}}(t') \rangle^{c} \\ = \sum_{\mathcal{P} \subset \mathcal{S}} (i\partial_{t} \langle \hat{A}_{\mathcal{P}}(t) \hat{B}_{\mathcal{P}}(t') \rangle^{c}) \sum_{\bigcup_{i} \mathcal{P}_{i} = \mathcal{S} \setminus \mathcal{P}} \prod_{\mathcal{P}_{i}} \langle \hat{A}_{\mathcal{P}_{i}}(t) \hat{B}_{\mathcal{P}_{i}}(t') \rangle^{c}.$$
(A.25)

Note that the partitions of S contain only *proper* subsets of S. The induction hypothesis is that the time derivative of $\langle \hat{A}_{\mathcal{P}}(t)\hat{B}_{\mathcal{P}}(t')\rangle^{c}$ can be expressed using (A.4)–(A.12) if \mathcal{P} is a proper subset of S. Substituting the first term in (A.4) to equation (A.25) leads to

$$(0') = \sum_{\mathcal{P} \subset \mathcal{S} \setminus \{\mu\}} \langle [\hat{A}_{\mathcal{P} \cup \{\mu\}}(t), \hat{H}_{\mu}(t)] \hat{B}_{\mathcal{P} \cup \{\mu\}}(t') \rangle \\ \times \sum_{\bigcup_{i} \mathcal{P}_{i} = \mathcal{S} \setminus \mathcal{P} \cup \{\mu\}} \prod_{\mathcal{P}_{i}} \langle \hat{A}_{\mathcal{P}_{i}}(t) \hat{B}_{\mathcal{P}_{i}}(t') \rangle^{c}, \qquad (A.26)$$

which is expression (A.14) without the summand $\mathcal{P} = \mathcal{S} \setminus \{\mu\}$. Therefore we find

$$(0) - (0') = \sum_{\mu \in \mathcal{S}} \langle [\hat{A}_{\mathcal{S}}(t), \hat{H}_{\mu}(t)] \hat{B}_{\mathcal{S}}(t') \rangle^{c}.$$
(A.27)

The contribution of the second term in (A.4) to equation (A.25) gives

$$(1') = -\frac{J}{Z} \sum_{\mathcal{P} \subset \mathcal{S}} \sum_{\mu,\nu \in \mathcal{P}} T_{\mu\nu} \langle [\hat{A}_{\mathcal{P}}(t), \hat{X}^{\dagger}_{\mu}(t) \hat{X}_{\nu}(t)] \hat{B}_{\mathcal{P}}(t') \rangle^{c} \\ \times \sum_{\bigcup_{i} \mathcal{P}_{i} = \mathcal{S} \setminus \mathcal{P}} \prod_{\mathcal{P}_{i}} \langle \hat{A}_{\mathcal{P}_{i}}(t) \hat{B}_{\mathcal{P}_{i}}(t') \rangle^{c}.$$
(A.28)

In equation (A.28), the term $\mathcal{P} = \mathcal{S}$ is excluded from the summation, contrary to equation (A.15), thus

$$(1) - (1') = -\frac{J}{Z} \sum_{\mu,\nu\in\mathcal{S}} T_{\mu\nu} \langle [\hat{A}_{\mathcal{S}}(t), \hat{X}^{\dagger}_{\mu}(t) \hat{X}_{\nu}(t)] \hat{B}_{\mathcal{S}}(t') \rangle^{c}.$$
(A.29)

The term (A.8) together with (A.25) leads to

$$(2a') = -\frac{J}{Z} \sum_{\mathcal{P} \subset \mathcal{S}} \sum_{\mu,\nu \in \mathcal{P}} \sum_{\mathcal{Q} \subseteq \mathcal{P} \setminus \{\mu,\nu\}} T_{\mu\nu} \langle [\hat{A}_{\mathcal{Q} \cup \{\mu\}}(t), \hat{X}^{\dagger}_{\mu}(t)] \hat{B}_{\mathcal{Q} \cup \{\mu\}}(t') \rangle^{c} \\ \times \langle \hat{X}_{\nu}(t) \hat{A}_{\bar{\mathcal{Q}} \cup \{\nu\}}(t) \hat{B}_{\bar{\mathcal{Q}} \cup \{\nu\}}(t') \rangle^{c} \sum_{\bigcup_{i} \mathcal{P}_{i} = \mathcal{S} \setminus \mathcal{P}} \prod_{\mathcal{P}_{i}} \langle \hat{A}_{\mathcal{P}_{i}}(t) \hat{B}_{\mathcal{P}_{i}}(t') \rangle^{c}.$$
(A.30)

Using the same reasoning as above we find the difference

$$(2a) - (2a') = -\frac{J}{Z} \sum_{\mu,\nu\in\mathcal{S}} \sum_{\mathcal{Q}\subseteq\mathcal{S}\setminus\{\mu,\nu\}}^{\mathcal{Q}\cup\bar{\mathcal{Q}}=\mathcal{S}\setminus\{\mu,\nu\}} T_{\mu\nu} \langle [\hat{A}_{\mathcal{Q}\cup\{\mu\}}(t), \hat{X}^{\dagger}_{\mu}(t)] \hat{B}_{\mathcal{Q}\cup\{\mu\}}(t') \rangle^{c} \times \langle \hat{X}_{\nu}(t) \hat{A}_{\bar{\mathcal{Q}}\cup\{\nu\}}(t) \hat{B}_{\bar{\mathcal{Q}}\cup\{\nu\}}(t') \rangle^{c}.$$
(A.31)

The part (A.9) from the hierarchy together with (A.25) leads to

$$(2b') = -\frac{J}{Z} \sum_{\mathcal{P} \subset \mathcal{S}} \sum_{\mu,\nu \in \mathcal{P}} \sum_{\mathcal{Q} \subseteq \mathcal{P} \setminus \{\mu,\nu\}} T_{\mu\nu} \langle \hat{A}_{\mathcal{Q} \cup \{\mu\}}(t) \hat{X}^{\dagger}_{\mu}(t) \hat{B}_{\mathcal{Q} \cup \{\mu\}}(t') \rangle^{c} \\ \times \langle [\hat{A}_{\bar{\mathcal{Q}} \cup \{\nu\}}(t), \hat{X}_{\nu}(t)] \hat{B}_{\bar{\mathcal{Q}} \cup \{\nu\}}(t') \rangle^{c} \sum_{\bigcup_{i} \mathcal{P}_{i} = \mathcal{S} \setminus \mathcal{P}} \prod_{\mathcal{P}_{i}} \langle \hat{A}_{\mathcal{P}_{i}}(t) \hat{B}_{\mathcal{P}_{i}}(t') \rangle^{c}$$
(A.32)

which has to be subtracted from (2b),

$$(2b) - (2b') = -\frac{J}{Z} \sum_{\mu,\nu\in\mathcal{S}} T_{\mu\nu} \sum_{\mathcal{Q}\subseteq\mathcal{S}\setminus\{\mu,\nu\}}^{\mathcal{Q}\cup\bar{\mathcal{Q}}=\mathcal{S}\setminus\{\mu,\nu\}} \langle \hat{A}_{\mathcal{Q}\cup\{\mu\}}(t)\hat{X}^{\dagger}_{\mu}(t)\hat{B}_{\mathcal{Q}\cup\{\mu\}}(t')\rangle^{c} \times \langle [\hat{A}_{\bar{\mathcal{Q}}\cup\{\nu\}}(t),\hat{X}_{\nu}(t)]\hat{B}_{\bar{\mathcal{Q}}\cup\{\nu\}}(t')\rangle^{c}.$$
(A.33)

The contribution of the first term in (A.5) to equation (A.25) leads to

$$(3a') = -\frac{J}{Z} \sum_{\mathcal{P} \subset \mathcal{S}} \sum_{\kappa \notin \mathcal{P}} \sum_{\mu \in \mathcal{P}} T_{\mu\kappa} \langle \hat{X}^{\dagger}_{\kappa}(t) [\hat{A}_{\mathcal{P}}(t), \hat{X}_{\mu}(t)] \hat{B}_{\mathcal{P}}(t') \rangle^{c} \times \sum_{\bigcup_{i} \mathcal{P}_{i} = \mathcal{S} \setminus \mathcal{P}} \prod_{\mathcal{P}_{i}} \langle \hat{A}_{\mathcal{P}_{i}}(t) \hat{B}_{\mathcal{P}_{i}}(t') \rangle^{c}$$
(A.34)

whereas the first term of (A.10) together with (A.25) gives

$$(3a'') = \frac{J}{Z} \sum_{\mathcal{P} \subset \mathcal{S}} \sum_{\mu,\nu \in \mathcal{P}} \sum_{\mathcal{Q} \subseteq \mathcal{P} \setminus \{\mu,\nu\}}^{\mathcal{Q} \cup \bar{\mathcal{Q}} = \mathcal{P} \setminus \{\mu,\nu\}} T_{\mu\nu} \langle \hat{A}_{\mathcal{Q} \cup \{\nu\}}(t) \hat{B}_{\mathcal{Q} \cup \{\nu\}}(t') \rangle^{c} \\ \times \langle \hat{X}_{\nu}^{\dagger}(t) [\hat{A}_{\bar{\mathcal{Q}} \cup \{\mu\}}(t), \hat{X}_{\mu}(t)] \hat{B}_{\bar{\mathcal{Q}} \cup \{\mu\}}(t') \rangle^{c} \\ \times \sum_{\cup_{i} \mathcal{P}_{i} = \mathcal{S} \setminus \mathcal{P}} \prod_{\mathcal{P}_{i}} \langle \hat{A}_{\mathcal{P}_{i}}(t) \hat{B}_{\mathcal{P}_{i}}(t') \rangle^{c}.$$
(A.35)

Splitting the sum over lattice sites κ according to $\sum_{\kappa \notin \mathcal{P}} = \sum_{\kappa \notin \mathcal{S}} + \sum_{\kappa \in \mathcal{S} \setminus \mathcal{P}}$ and sub-tracting (3*a*') as well as (3*a*'') from (A.20) leads to

$$(3a) - (3a') - (3a'') = -\frac{J}{Z} \sum_{\kappa \notin S} \sum_{\mu \in S} T_{\mu\kappa} \langle \hat{X}^{\dagger}_{\kappa}(t) [\hat{A}_{\mathcal{S}}(t), \hat{X}_{\mu}(t)] \hat{B}_{\mathcal{S}}(t') \rangle^{c} + \frac{J}{Z} \sum_{\mu,\nu \in S} \sum_{\mathcal{P} \subseteq \mathcal{S} \setminus \{\mu,\nu\}}^{\mathcal{P} \cup \bar{\mathcal{P}} = \mathcal{S} \setminus \{\mu,\nu\}} T_{\mu\nu} \langle \hat{A}_{\mathcal{P} \cup \{\nu\}}(t) \hat{B}_{\mathcal{P} \cup \{\nu\}}(t') \rangle^{c} \times \langle \hat{X}^{\dagger}_{\nu}(t) [\hat{A}_{\bar{\mathcal{P}} \cup \{\mu\}}(t), \hat{X}_{\mu}(t)] \hat{B}_{\bar{\mathcal{P}} \cup \{\mu\}}(t') \rangle^{c}.$$
(A.36)

Similarly, we obtain from the second term in (A.5) the contribution

$$(3b') = -\frac{J}{Z} \sum_{\mathcal{P} \subset \mathcal{S}} \sum_{\kappa \notin \mathcal{P}} \sum_{\mu \in \mathcal{P}} T_{\mu\kappa} \langle \hat{X}_{\kappa}(t) [\hat{A}_{\mathcal{P}}(t), \hat{X}^{\dagger}_{\mu}(t)] \hat{B}_{\mathcal{P}}(t') \rangle^{c} \times \sum_{\bigcup_{i} \mathcal{P}_{i} = \mathcal{S} \setminus \mathcal{P}} \prod_{\mathcal{P}_{i}} \langle \hat{A}_{\mathcal{P}_{i}}(t) \hat{B}_{\mathcal{P}_{i}}(t') \rangle^{c}$$
(A.37)

and from the second term in (A.10) we have

$$(3b'') = \frac{J}{Z} \sum_{\mathcal{P} \subset \mathcal{S}} \sum_{\mu,\nu \in \mathcal{P}} \sum_{\mathcal{Q} \subseteq \mathcal{P} \setminus \{\mu,\nu\}}^{\mathcal{Q} \cup \bar{\mathcal{Q}} = \mathcal{P} \setminus \{\mu,\nu\}} T_{\mu\nu} \langle \hat{A}_{\mathcal{Q} \cup \{\nu\}}(t) \hat{B}_{\mathcal{Q} \cup \{\nu\}}(t') \rangle^{c} \\ \times \langle \hat{X}_{\nu}(t) [\hat{A}_{\bar{\mathcal{Q}} \cup \{\mu\}}(t), \hat{X}^{\dagger}_{\mu}(t)] \hat{B}_{\bar{\mathcal{Q}} \cup \{\mu\}}(t') \rangle^{c} \\ \times \sum_{\cup_{i} \mathcal{P}_{i} = \mathcal{S} \setminus \mathcal{P}} \prod_{\mathcal{P}_{i}} \langle \hat{A}_{\mathcal{P}_{i}}(t) \hat{B}_{\mathcal{P}_{i}}(t') \rangle^{c}.$$
(A.38)

Subtracting these expressions from equation (A.23) leads to

$$(3b) - (3b') - (3b'') = -\frac{J}{Z} \sum_{\kappa \notin S} \sum_{\mu \in S} T_{\mu\kappa} \langle \hat{X}_{\kappa}(t) [\hat{A}_{\mathcal{S}}(t), \hat{X}^{\dagger}_{\mu}(t)] \hat{B}_{\mathcal{S}}(t') \rangle^{c} + \frac{J}{Z} \sum_{\mu,\nu \in S} \sum_{\mathcal{P} \subseteq \mathcal{S} \setminus \{\mu,\nu\}}^{\mathcal{P} \cup \bar{\mathcal{P}} = \mathcal{S} \setminus \{\mu,\nu\}} T_{\mu\nu} \langle \hat{A}_{\mathcal{P} \cup \{\nu\}}(t) \hat{B}_{\mathcal{P} \cup \{\nu\}}(t') \rangle^{c} \times \langle \hat{X}_{\nu}(t) [\hat{A}_{\bar{\mathcal{P}} \cup \{\mu\}}(t), \hat{X}^{\dagger}_{\mu}(t)] \hat{B}_{\bar{\mathcal{P}} \cup \{\mu\}}(t') \rangle^{c}.$$
(A.39)

The contribution of (A.6) gives

$$(4a') = -\frac{J}{Z} \sum_{\mathcal{P} \subset \mathcal{S}} \sum_{\kappa \notin \mathcal{P}} \sum_{\mu \in \mathcal{P}} \sum_{\mathcal{Q} \subseteq \mathcal{P} \setminus \{\mu\}} T_{\mu\kappa} \langle [\hat{A}_{\mathcal{Q} \cup \{\mu\}}(t), \hat{X}_{\mu}(t)] \hat{B}_{\mathcal{Q} \cup \{\mu\}}(t') \rangle^{c} \times \langle \hat{X}_{\kappa}^{\dagger}(t) \hat{A}_{\bar{\mathcal{Q}}}(t) \hat{B}_{\bar{\mathcal{Q}}}(t') \rangle^{c} \sum_{\cup_{i} \mathcal{P}_{i} = \mathcal{S} \setminus \mathcal{P}} \prod_{\mathcal{P}_{i}} \langle \hat{A}_{\mathcal{P}_{i}}(t) \hat{B}_{\mathcal{P}_{i}}(t') \rangle^{c}$$
(A.40)

whereas from (A.11) we obtain the contribution

$$(4a'') = \frac{J}{Z} \sum_{\mathcal{P} \subset \mathcal{S}} \sum_{\mu,\nu \in \mathcal{P}} \sum_{\mathcal{R} \subseteq \mathcal{P} \setminus \{\mu,\nu\}}^{\mathcal{R} \cup \bar{\mathcal{R}} = \mathcal{P} \setminus \{\mu,\nu\}} T_{\mu\nu} \langle \hat{A}_{\mathcal{R} \cup \{\nu\}}(t) \hat{B}_{\mathcal{R} \cup \{\nu\}}(t') \rangle^{c} \\ \times \sum_{\mathcal{Q} \subseteq \bar{\mathcal{R}}}^{\mathcal{Q} \cup \bar{\mathcal{Q}} = \bar{\mathcal{R}}} \langle [\hat{A}_{\mathcal{Q} \cup \{\mu\}}(t), \hat{X}_{\mu}(t)] \hat{B}_{\mathcal{Q} \cup \{\mu\}}(t') \rangle^{c} \langle \hat{X}_{\nu}^{\dagger}(t) \hat{A}_{\bar{\mathcal{Q}}}(t) \hat{B}_{\bar{\mathcal{Q}}}(t') \rangle^{c} \\ \times \sum_{\cup_{i} \mathcal{P}_{i} = \mathcal{S} \setminus \mathcal{P}} \prod_{\mathcal{P}_{i}} \langle \hat{A}_{\mathcal{P}_{i}}(t) \hat{B}_{\mathcal{P}_{i}}(t') \rangle^{c}.$$
(A.41)

(4a') and (4a'') from relation (A.21) leads to

$$(4a) - (4a') - (4a'') = -\frac{J}{Z} \sum_{\kappa \notin \mathcal{S}} \sum_{\mu \in \mathcal{S}} T_{\mu\kappa} \sum_{\mathcal{P} \subseteq \mathcal{S} \setminus \{\mu\}}^{\mathcal{P} \cup \bar{\mathcal{P}} = \mathcal{S} \setminus \{\mu\}} \langle [\hat{A}_{\mathcal{P} \cup \{\mu\}}(t), \hat{X}_{\mu}(t)] \hat{B}_{\mathcal{P} \cup \{\mu\}}(t') \rangle^{c} \\ \times \langle \hat{X}_{\kappa}^{\dagger}(t) \hat{A}_{\bar{\mathcal{P}}}(t) \hat{B}_{\bar{\mathcal{P}}}(t') \rangle^{c}$$

$$+ \frac{J}{Z} \sum_{\mu\nu\in\mathcal{S}} \sum_{\mathcal{P}\subseteq\mathcal{S}\setminus\{\mu,\nu\}}^{\mathcal{P}\cup\bar{\mathcal{P}}=\mathcal{S}\setminus\{\mu,\nu\}} T_{\mu\nu} \sum_{\mathcal{Q}\subseteq\bar{\mathcal{P}}}^{\mathcal{Q}\cup\bar{\mathcal{Q}}=\bar{\mathcal{P}}} \langle [\hat{A}_{\mathcal{Q}\cup\{\mu\}}(t), \hat{X}_{\mu}(t)] \hat{B}_{\mathcal{Q}\cup\{\mu\}}(t') \rangle^{c} \\ \times \langle \hat{X}_{\nu}^{\dagger}(t) \hat{A}_{\bar{\mathcal{Q}}}(t) \hat{B}_{\bar{\mathcal{Q}}}(t') \rangle^{c} \langle \hat{A}_{\mathcal{P}\cup\{\nu\}}(t) \hat{B}_{\mathcal{P}\cup\{\nu\}}(t') \rangle^{c}.$$
(A.42)

From (A.7) we get the term

$$(4b') = -\frac{J}{Z} \sum_{\mathcal{P} \subset \mathcal{S}} \sum_{\kappa \notin \mathcal{P}} \sum_{\mu \in \mathcal{P}} \sum_{\mathcal{Q} \subseteq \mathcal{P} \setminus \{\mu\}} \sum_{\mathcal{Q} \subseteq \mathcal{P} \setminus \{\mu\}} T_{\mu\kappa} \langle [\hat{A}_{\mathcal{Q} \cup \{\mu\}}(t), \hat{X}^{\dagger}_{\mu}(t)] \hat{B}_{\mathcal{Q} \cup \{\mu\}}(t') \rangle^{c} \\ \times \langle \hat{X}_{\kappa}(t) \hat{A}_{\bar{\mathcal{Q}}}(t) \hat{B}_{\bar{\mathcal{Q}}}(t') \rangle^{c} \sum_{\cup_{i} \mathcal{P}_{i} = \mathcal{S} \setminus \mathcal{P}} \prod_{\mathcal{P}_{i}} \langle \hat{A}_{\mathcal{P}_{i}}(t) \hat{B}_{\mathcal{P}_{i}}(t') \rangle^{c}$$
(A.43)

and from equation (A.12) originates

$$(4b'') = \frac{J}{Z} \sum_{\mathcal{P} \subset \mathcal{S}} \sum_{\mu,\nu \in \mathcal{P}} \sum_{\mathcal{R} \subseteq \mathcal{P} \setminus \{\mu,\nu\}}^{\mathcal{R} \cup \bar{\mathcal{R}} = \mathcal{P} \setminus \{\mu,\nu\}} T_{\mu\nu} \langle \hat{A}_{\mathcal{R} \cup \{\nu\}}(t) \hat{B}_{\mathcal{R} \cup \{\nu\}}(t') \rangle^{c}$$

$$\times \sum_{\mathcal{Q} \subseteq \bar{\mathcal{R}}} \sum_{\mathcal{Q} \subseteq \bar{\mathcal{R}}} \langle [\hat{A}_{\mathcal{Q} \cup \{\mu\}}(t), \hat{X}^{\dagger}_{\mu}(t)] \hat{B}_{\mathcal{Q} \cup \{\mu\}}(t') \rangle^{c} \langle \hat{X}_{\nu}(t) \hat{A}_{\bar{\mathcal{Q}}}(t) \hat{B}_{\bar{\mathcal{Q}}}(t') \rangle^{c}$$

$$\times \sum_{\cup_{i} \mathcal{P}_{i} = \mathcal{S} \setminus \mathcal{P}} \prod_{\mathcal{P}_{i}} \langle \hat{A}_{\mathcal{P}_{i}}(t) \hat{B}_{\mathcal{P}_{i}}(t') \rangle^{c}. \qquad (A.44)$$

After subtracting these terms from (A.24) we have

$$(4b) - (4b') - (4b'')$$

$$= -\frac{J}{Z} \sum_{\kappa \notin S} \sum_{\mu \in S} T_{\mu\kappa} \sum_{\mathcal{P} \subseteq S \setminus \{\mu\}}^{\mathcal{P} \cup \bar{\mathcal{P}} = S \setminus \{\mu\}} \langle [\hat{A}_{\mathcal{P} \cup \{\mu\}}(t), \hat{X}^{\dagger}_{\mu}(t)] \hat{B}_{\mathcal{P} \cup \{\mu\}}(t') \rangle^{c}$$

$$\times \langle \hat{X}_{\kappa}(t) \hat{A}_{\bar{\mathcal{P}}}(t) \hat{B}_{\bar{\mathcal{P}}}(t') \rangle^{c}$$

$$+ \frac{J}{Z} \sum_{\mu\nu \in S} \sum_{\mathcal{P} \subseteq S \setminus \{\mu,\nu\}}^{\mathcal{P} \cup \bar{\mathcal{P}} = S \setminus \{\mu,\nu\}} T_{\mu\nu} \sum_{\mathcal{Q} \subseteq \bar{\mathcal{P}}}^{\mathcal{Q} \cup \bar{\mathcal{Q}} = \bar{\mathcal{P}}} \langle [\hat{A}_{\mathcal{Q} \cup \{\mu\}}(t), \hat{X}^{\dagger}_{\mu}(t)] \hat{B}_{\mathcal{Q} \cup \{\mu\}}(t') \rangle^{c}$$

$$\times \langle \hat{X}_{\nu}(t) \hat{A}_{\bar{\mathcal{Q}}}(t) \hat{B}_{\bar{\mathcal{Q}}}(t') \rangle^{c} \langle \hat{A}_{\mathcal{P} \cup \{\nu\}}(t) \hat{B}_{\mathcal{P} \cup \{\nu\}}(t') \rangle^{c}. \qquad (A.45)$$

Adding the equations (A.27), (A.29), (A.31), (A.33), (A.36), (A.39), (A.42) and (A.45) together leads to the right hand side of the hierarchy (A.4)–(A.12) for a set with cardinality |S|. This completes the proof.

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