The Structure of Operators in Effective Particle-Conserving Models

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I. INTRODUCTION

Effective models are at the very center of theoretical physics since they allow to focus on the essential physics of a problem without being distracted by unnecessary complexity. Hence it is very important to dispose of systematic means to derive effective models. Here we will present the mathematical structure of a certain kind of effective models, namely effective models where the elementary excitations above the ground state can be viewed as particles above a complex vacuum. This type of view is very common in low-temperature physics. Many experiments can be understood on the basis of this picture.

In this paper, we will elucidate the global structure of the Hamiltonian and of the observables if the model is transformed to a model which conserves the number of particles. Such a mapping is often possible and renders the subsequent calculation of physical quantities much easier. The determination of the effective Hamiltonian is facilitated by the decomposition into $n$-particle irreducible parts. We set up such a classification at zero temperature for strong-coupling situations, i.e. no weak-coupling limit is needed and no non-interacting fermions or bosons are required. Generically, we deal with hard-core bosons.

The necessity for the decomposition into $n$-particle irreducible parts has arisen in perturbative calculations of the effective Hamiltonians because only the $n$-particle irreducible interactions are independent of the system size. The second main point of this article is the perturbative computation of effective Hamiltonians and observables. Such computations are a standard technique for ground state energies (0-particle terms) and dispersion relations (1-particle terms), see Ref. [1] and references therein. But the possibility to compute multi-particle contributions has only recently been realized [2–4] and continues to be exploited intensively. The key ingredient is to define a similarity transformation on the operator level (see below).

A promising alternative route, which we can only sketch in this article, consists in the non-perturbative, renormalizing realization of the transformation of the initial model to the effective model which conserved the number of particles. Examples of this approach are realized in fermionic models [5–7].

A. Starting point

We consider models which are defined on a lattice $\Gamma$. At each site of the lattice the system can be in a number $d$ of states spanning the local Hilbert space. Let us assume that $d$ is finite. The dynamics of the system is governed by a Hamiltonian $H$ acting in the tensor-product space of the local Hilbert spaces. For simplicity we do not consider antisymmetric, fermionic situations although this is also possible. So we are focusing on physical systems which can be described in terms of hard-core bosons.

The Hamiltonian $H$ is assumed to be of finite range. This means that it is composed of local operators $h_\nu$ acting on a finite number of sites in the vicinity of the site $\nu$.

$$H = \sum_{\nu} h_\nu .$$ (1)

We further assume, that $H$ can be split as

$$H(x) = U + xV ,$$ (2)

so that the spectrum of $U$ is simple (see below) and that the system does not undergo a phase transition from $x = 0$ to the range of values we are finally interested in. These requirements do not necessarily imply that $x$ has to be small. But it is helpful if this is the case.

The ground state of $U$ and its lowest lying eigen-states shall be known. The latter will be viewed as elementary excitations from which the whole spectrum can be built. We assume that we can view the elementary excitations above the ground state as (quasi-)particles above the vacuum. For simplicity, we will drop the prefix ‘quasi-’: it is understood that ‘particle’ is a synonym for elementary excitation.
We assume that the physical picture sketched for $H(x = 0) = U$ is linked continuously to the range $0 \leq x \leq x_c$ where $x_c$ is the critical value at which a phase transition occurs. At the critical value $x_c$ the picture breaks down and cannot be used beyond $x = x_c$. Generically, a mode of $H(x)$ will become soft at $x_c$.

Furthermore, the particles for $x = 0$ shall be local in the sense that we can assign a site to each of them. Let $Q$ be the operator that counts the number of particles.

As a concrete example, the reader may think of an antiferromagnetic Heisenberg model made up from strongly coupled (coupling $J$) pairs of spins (‘dimers’) which are weakly coupled (coupling $xJ$) among themselves, e.g. $[3,8]$. At $x = 0$, the ground state is the product state with singlets on all dimers; the elementary excitations are local triplets. The number of these local triplets, i.e. the number of dimers which are not in the singlet state, shall be given by the operator $Q$.

A considerable simplification of the problem can be achieved by mapping the initial problem $H(x)$ to an effective Hamiltonian $H_{\text{eff}}(x)$ in which the number of elementary excitations does not change. That is the number of particles should be a conserved quantity. Then the computation of many physical quantities is significantly simplified.

In this article, we advocate to use a continuous unitary transformation (CUT) $[9–11,8]$ in order to achieve a systematically controlled mapping of the kind described above which leads to

$$[H_{\text{eff}}, Q] = 0 ,$$

i.e. $H_{\text{eff}}$ conserves the number of particles. Such an approach has three major advantages:

1. Conceptual clarity
   Using a unitary transformation guarantees that no information of the original model is lost. In particular, it is clear that the same transformation $[9,12–14]$ can be applied to obtain the effective observables $O_{\text{eff}}$ from the original observables $O$.

2. Technical simplicity
   To implement the unitary transformation in a continuous fashion only the computation of commutators is required since the mapping is split into infinitesimal steps leading to a differential equation [9]

$$\partial_\ell H = [\eta(\ell), H(\ell)]$$

where $\ell \in [0, \infty]$ is an auxiliary parameter parametrizing the continuous transformation with starting point $\ell = 0$ and end point $\ell = \infty$.

3. Good controllability
   By an appropriate choice of the infinitesimal generator $\eta$ of the transformation it can be designed such that is preserves block-band diagonality $[8,11]$.

Moreover, it is renormalizing in the sense that matrix elements between energetically very different states are transformed more rapidly than those between energetically adjacent states $[5,6,11]$.

We like to point out, however, that the general structure of operators does not depend on the details of the method by which the effective particle-conserving model is obtained. Also other methods than CUTs are conceivable.

In the present paper we will focus on perturbative realizations of the CUTs. This approach $[8]$ was the first which realized the computation of bound states in higher orders $[2,3]$. The concept of a similarity transformation is indispensable for a conceptually clear computation of multi-particle effects $[4,15]$.

**B. Setup**

In Sect. II we analyse global structural aspects of effective operators. The basic prerequisite will be Eq. (3). Furthermore, we show that the linked cluster property holds. Therefore the effective operators which hold in the thermodynamic limit can be computed in finite systems.

Sect. III is a preparatory section in which the perturbative CUT for Hamilton operators of certain kind is constructed. Low-dimensional spin models on lattices are among the models which can be treated in this way.

Sect. IV contains a detailed description of how the perturbative CUT can be extended to transform general observables. Series expansions in $x$ for the effective observables are obtained which allow to compute the experimentally relevant spectral functions. So the extension from Hamiltonians to observables is an important one.

The article is concluded in Sect. V.

**II. THE STRUCTURE OF EFFECTIVE OPERATORS**

In this section, we assume that we are able to construct a mapping such that $H_{\text{eff}}$ fulfills Eq. (3). The eigen-states of the particle number operator $Q$ serve as a basis for the Hilbert space of the system. If the mapping is realized perturbatively, the matrix elements of $H_{\text{eff}}$ and $O_{\text{eff}}$ are polynomials in $x$.

**A. The effective Hamiltonian**

1. Global structure

We will show that $H_{\text{eff}}$ can be written as

$$H_{\text{eff}} = H_0 + H_1 + H_2 + H_3 + \ldots ,$$

(5)
where $H_n$ is an $n$-particle irreducible operator, i.e. $H_n$ measures $n$-particle energies. Moreover, each thermodynamic matrix element of any of the components $H_n$ can be obtained on finite clusters for a given order in $x$ if the original Hamiltonian is of finite range. The components $H_n$ can be defined recursively in ascending order in $n$.

Eq. (5) comprises already a route to determine the properties of $H_{\text{eff}}$ in a sequence of approximate treatments. The very first step is to know the ground state which defines $H_0$. The second level is to describe the dynamics of a single particle (elementary excitations) correctly which is possible by knowing $H_1$. The third level is reached if $H_2$ is included which contains the information on the interaction of two particles. True three-particle interactions are contained in $H_3$ and so on. From the generic experience in condensed matter theory, the three- and more particle terms can very often be neglected. So the first three terms in Eq. (5) provide the systematically controlled starting point of a broad class of problems.

Let us clarify some notation. We define the following eigen-states of the particle number operator $Q$

\[
\begin{align*}
|0\rangle & \text{ ground state (particle vacuum)} \\
|i\rangle & \text{ state with 1 particle on site } i \\
|i_1i_2\rangle & \text{ state with 2 particles on sites } i_1 \text{ and } i_2 \\
& \vdots
\end{align*}
\]

i.e. $Q|0\rangle = 0|0\rangle$, $Q|i\rangle = 1|i\rangle$ and $Q|i\rangle = 2|i\rangle$ and so on. These states span the global Hilbert space $\mathcal{E}$ of the physical system under study. Dealing with (hard-core) bosons $|i_1i_2\rangle$ and $|i_2i_1\rangle$ are identical states. This indistinguishability causes a certain ambiguity. This ambiguity can be remedied for instance by assuming that coefficients depending on several indices $i_1i_2 \ldots i_n$ are even under permutation of any pair of these indices [16]. For simplicity, the ground state $|0\rangle$ is assumed to be unique.

Let $\mathcal{R}$ be an arbitrary operator acting on $\mathcal{E}$ and conserving the number of particles $[\mathcal{R},Q] = 0$. By $\mathcal{R}|n\rangle$ we denote the restricted operator acting on $\mathcal{E}_n \subset \mathcal{E}$ spanned by all states with exactly $n$ particles.

Now we define the operators $H_n$

\[
\begin{align*}
H_0 & := E_01 \\
H_1 & := \sum_{ij} t_{ij} e_{ij}^\dagger e_i \\
H_2 & := \sum_{i_1i_2j_1j_2} t_{j_1j_2;i_1i_2} e_{j_1}^\dagger e_{j_2}^\dagger e_{i_1} e_{i_2} \\
& \vdots \\
H_n & := \sum_{i_1 \ldots i_nj_1 \ldots j_n} t_{j_1 \ldots j_n;i_1 \ldots i_n} e_{j_1}^\dagger \ldots e_{j_n}^\dagger e_{i_1} \ldots e_{i_n}.
\end{align*}
\]

where $1$ is the identity operator. Note that these operators are defined on the full Hilbert space $\mathcal{E}$. The operators $e_i^\dagger$ are local operators that annihilate (create) particles at site $i$. They are bosonic operators. Their definition can be tailored to include a hard-core repulsion between the particles to account for the common situation that at maximum one of the particles may be present at given site $i$. If the particles have additional internal quantum numbers, i.e. if there can be different particles at each site, the indices $i$ and $j$ are substituted by multi-indices $1$ and $j$.

As an example let us consider that there are three kinds of particles per sites, but that at maximum one of these particles can occupy a given site. Then each site corresponds to a four-level system; the particles are hard-core bosons. Such a situation arises in antiferromagnetic dimerized spin systems where each dimer represents a four-level system. The ground state is the unique singlet while the three particles are given by the three-fold degenerate triplet states. In this case we have the multi-indices $i = (i_1, \alpha)$, where $i$ denotes the site and $\alpha$ takes for instance the three values of the $S^z$ component $\alpha \in \{-1, 0, 1\}$. In the local basis $\{|i, s\rangle, |i, -1\rangle, |i, 0\rangle, |i, 1\rangle\}$, where $s$ denotes the singlet, the local creation operators $e_{i,\alpha}^\dagger$ are the $4 \times 4$-matrices

\[
\begin{align*}
e_{i,1}^\dagger & = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, & (8a) \\
e_{i,0}^\dagger & = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, & (8b) \\
e_{i,-1}^\dagger & = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}. & (8c)
\end{align*}
\]

It is understood that the action at all other sites but $i$ is the identity so that the operators in (8) are defined on the whole Hilbert space. The annihilation operators $e_{i,\alpha}$ are given by the hermitian conjugate matrices. All possible commutators can easily be computed within the matrix representation. Finite matrix elements in the lower right $3 \times 3$ block can be viewed as combined annihilation & creation processes: The matrix $M_{\alpha,\beta}$ with all elements zero except the one at $(\alpha, \beta)$ corresponds to the process $e_{i,\alpha}^\dagger e_{i,\beta}$. A finite matrix element in the upper left $1 \times 1$ block, i.e. the singlet-singlet channel, can be expressed in normal-ordered fashion as $1_4 - \sum_{\alpha} e_{i,\alpha}^\dagger e_{i,\alpha}$. In this way the operators (8) and their hermitian conjugate define a complete algebra which in turn enables us to classify contributions of the Hamiltonian according to the number of particles affected as done in Eqs. (5) and (7).

The decomposition (5) is physically very intuitive. Yet the next important question is whether and how the operators $H_n$ are unambiguously defined. This issue is addressed by noting that $H_n|m\rangle$ vanishes for $m < n$. This follows directly from the normal-ordering of the creation
and annihilation operators in Eq. (7). Then we can proceed iteratively by requiring that $H_{\text{eff}}$ applied to $n$ particles corresponds to $H_0 + H_1 + \ldots + H_n$ (arbitrary but fixed). Solving for $H_n$ yields the recursions
\begin{align}
H_0 |0\rangle &= H_{\text{eff}} |0\rangle \quad (9a) \\
H_1 |1\rangle &= H_{\text{eff}} |1\rangle - H_0 |1\rangle \quad (9b) \\
H_2 |2\rangle &= H_{\text{eff}} |2\rangle - H_0 |2\rangle - H_1 |2\rangle \quad (9c) \\
&\vdots \\
H_n |n\rangle &= H_{\text{eff}} |n\rangle - \sum_{i=0}^{n-1} H_i |n\rangle. \quad (9d)
\end{align}

Assuming that $H_{\text{eff}}$ is calculated beforehand one starts by evaluating $E_0$ by means of the first definition. The result entirely defines $H_0$. The restriction $H_0|1\rangle$ is then used in the second equation to extract the $t_{ij}$ of $H_1$ and so on. Generally, $H_n$ is defined on the full many-particle Hilbert space, not only for $n$ particles. But it is sufficient to know the action of $H_n$ on the subspace of $n$ particles to determine all its matrix elements in (7). It is the essential merit of the notation in second quantization (7) that it provides the natural generalization of the action of a part of the Hamiltonian on a finite number of particles to an arbitrary number of particles. Since Eq. (9d) holds for any number of particles and since $H_n|n\rangle$ vanishes for $m < n$ we obtain Eq. (5), neglecting the precise definition of convergence which is beyond the scope of the present paper.

In conventional many-body language, $H_n$ stands for the $n$-particle irreducible interaction. The subtractions in Eq. (9) ensure that $H_n$ contains no reducible contributions, i.e. contributions which really act only on a lower number of particles. It should be emphasized that the formalism above does not require that a simple free fermionic or bosonic limit exists. It is possible to start from any type of elementary particles counted by some operator $Q$.

Moreover, the formalism presented in this section does not depend on how $H_{\text{eff}}$ is obtained. It does not matter whether a perturbative, a renormalizing procedure or a rigorously exact method was used to obtain $H_{\text{eff}}$.

2. Cluster additivity

Here we focus on formal aspects of a perturbative approach generalizing results obtained previously for 0-particle properties [17] and for 1-particle properties [18]. The feature that the Hamiltonian is of finite range on the lattice is exploited. Then the Eqs. (9) can be evaluated on finite subsystems (clusters, see below). Still, the thermodynamically relevant matrix elements of the operators $H_n$ are obtained as we show in the following paragraphs.

To proceed further definitions are needed. A cluster $C$ of the thermodynamic system is a finite subset of sites of the system and their linking bonds. By $C^C$ we denote an operator which acts only on the Hilbert space $\mathcal{E}^C$ of $C$. If $C$ denotes the sites of the total system which are not included in $C$, the restricted operator $\mathcal{R}^C$ is lifted naturally to an operator $\mathcal{R}$ in the total Hilbert space $\mathcal{E} = \mathcal{E}^C \otimes \mathcal{E}^C$ by
\begin{align}
\mathcal{R} := \mathcal{R}^C \otimes 1^C. 
\end{align}

Note that it is not possible to define a restricted operator $\mathcal{R}^C$ from an arbitrary operator $\mathcal{R}$ acting on $\mathcal{E}$ since $\mathcal{R}$ will not have the product structure (10) in general.

Two clusters $A$ and $B$ are said to form a disconnected cluster $C = A \cup B$ iff they do not have any site in common $A \cap B = 0$ and there is no bond linking sites from $A$ with sites from $B$. Otherwise the clusters $A$ and $B$ are said to constitute together a linked cluster $C = A \cup B$. Given a disconnected cluster $C = A \cup B$ an operator $\mathcal{R}^C$ is called cluster additive if it can be decomposed as
\begin{align}
\mathcal{R}^C = \mathcal{R}^A \otimes 1^B + 1^A \otimes \mathcal{R}^B.
\end{align}

With these definitions we show that $H_{\text{eff}}$ and $H_n$ are cluster additive. But $H_{\text{eff}}|n\rangle$ is not! This will turn out to be another important reason to introduce the $H_n$.

The cluster additivity of $H_{\text{eff}}^C$ is obvious since $A$ and $B$ are assumed to be disconnected. So they can be viewed as physically independent systems. Hence
\begin{align}
H_{\text{eff}}^C = H_n^A \otimes 1^B + 1^A \otimes H_n^B.
\end{align}

Similarly, we deduce from (9) the operators $H_n^A$ and $H_n^B$ which act on $\mathcal{E}^A$ and $\mathcal{E}^B$, respectively. Then it is straightforward to verify that the operators
\begin{align}
H_n^C = H_n^A \otimes 1^B + 1^A \otimes H_n^B
\end{align}
fulfil the recursion (9) for the operators defined for the cluster $C$. Hence the operators $H_{\text{eff}}$ and $H_n$ are indeed cluster additive.

It is instructive to see that $H_{\text{eff}}|n\rangle$ is not cluster additive, contrary to what one might have thought. Let us consider the tentative identity
\begin{align}
H_{\text{eff}}^C|n\rangle = H_n^A \otimes 1^B + 1^A \otimes H_n^B|n\rangle.
\end{align}

This equation cannot be true since on the left hand side the number of particles is fixed to $n$ while on the right hand side the number of particles to which the identities $1^A$ and $1^B$ are applied is not fixed. So no cluster additivity is given for the $H_{\text{eff}}|n\rangle$.

The fact that cluster additivity holds only for particular quantities was noted previously for $n = 1$ [18]. For $n = 2$, the subtraction procedure was first applied in the calculations in Ref. [2] (though not given in detail). In Refs. [3,4,15,22] the subtractions necessary to obtain the irreducible 2-particle interaction were given in more detail. The general formalism presented in this article shows on the operator level why such subtractions are
necessary and where they come from. Thereby, it is possible to extend the treatment to the general n-particle irreducible interaction.

The notation in terms of second quantization (7) renders the cluster additivity almost trivial. This is so since the creation and annihilation operators are defined locally for a certain site. It is understood that the other sites are not affected. Hence the same symbol \( e_i \) can be used independent of the cluster in which the site \( i \) is embedded. In particular, one identifies automatically \( e_i^\dagger \otimes 1_B \) if \( i \in A \) and with \( 1_A \otimes e_i^\dagger \otimes 1_B \) if \( i \in B \). Hence cluster additivity is reduced to trivial statements of the kind that

\[
H_1^A = \sum_{i,j \in A} t_{ji} e_j^\dagger e_i^\dagger \quad (15a)
\]

\[
H_1^B = \sum_{i,j \in B} t_{ji} e_j^\dagger e_i^\dagger \quad (15b)
\]

implies

\[
H_1^C = \sum_{i,j \in C} t_{ji} e_j^\dagger e_i^\dagger = \sum_{i,j \in A} t_{ji} e_j^\dagger e_i^\dagger + \sum_{i,j \in B} t_{ji} e_j^\dagger e_i^\dagger = H_1^A \otimes 1_B + 1_A \otimes H_1^B. \quad (16c)
\]

In this sense, the notation in second quantization is the most natural way to think of cluster additivity.

Following Gelfand and co-workers [1,17,18] we conclude that the cluster additive quantities possess a cluster expansion. Hence all the irreducible matrix elements \( t_{ji} \) possess a cluster expansion and can be computed on finite clusters.

### 3. Computational aspects

Since \( H_{\text{eff}} \) conserves the number of particles, i.e., Eq. (3), its action is to shift existing particles. Let us denote the relevant matrix elements for a linked cluster \( A \) by

\[
E_0^A := \langle 0 | H_{\text{eff}}^A | 0 \rangle \quad (17a)
\]

\[
a_{ji}^A := \langle j | H_{\text{eff}}^A | i \rangle \quad (17b)
\]

\[
a_{j_1,j_2; i_1,i_2}^A := \langle j_1,j_2 | H_{\text{eff}}^A | i_1,i_2 \rangle \quad (17c)
\]

where the indices \( i,j, \ldots \) may be multi-indices from now on. Put differently, \( E_0^A \) is the matrix element of \( H_{\text{eff}}^A \), the \( a_{ji}^A \) are the matrix elements of \( H_{\text{eff}}^A | 1 \), the \( a_{j_1,j_2; i_1,i_2}^A \) of \( H_{\text{eff}}^A | 2 \) and so on. The number \( E_0^A \) is the ground state energy of cluster \( A \). The recursive definitions (9) imply

\[
t_{j_1,i}^A = a_{j_1,i}^A = E_0^A \delta_{ji} \quad (18a)
\]

\[
t_{j_1,j_2;i_1,i_2}^A = a_{j_1,j_2;i_1,i_2}^A = E_0^A \delta_{j_1,i_1} \delta_{j_2,i_2} - E_0^A \delta_{j_1,i_2} \delta_{j_2,i_1} - t_{j_2,i_2}^A \delta_{j_1,i_1} - t_{j_1,i_2}^A \delta_{j_1,i_2} - t_{j_1,i_1}^A \delta_{j_2,i_2} \quad (18b)
\]

\[
t_{j_1,j_2;j_3;i_1,i_2,i_3}^A = a_{j_1,j_2;j_3;i_1,i_2,i_3}^A = A_0 - A_1 - A_2 \quad (18c)
\]

where \( A_0 \) comprises six terms resulting from \( H_0 \), \( A_1 \) comprises 18 terms resulting from \( H_1 \) and \( A_2 \) comprises 36 terms resulting from \( H_2 \). The explicit formulae are given in Appendix A. The recipe in deriving the above equations is straightforward. For a given \( n \)-particle process \( \{i_m\} \to \{j_m\} (m \in \{1, \ldots, n\}) \) one has to subtract all possible processes which move less than \( n \) particles. Since the \( m \)-particle processes with \( m < n \) have been computed before the procedure is recursive. Note that all coefficients must be computed for the same cluster.

The cluster additivity or, equivalently, the existence of a cluster expansion can be exploited to compute the irreducible matrix elements on finite clusters given that the Hamiltonian is of finite range. There are two strategies to do so.

The first strategy is to choose a cluster large enough to perform the intended computation without finite-size effects. This strategy works particularly well if the dimensionality of the problem is low. Let us assume for simplicity that the Hamiltonian links only nearest-neighbour sites. Aiming at a given matrix element, for instance \( t_{j_1,j_2;i_1,i_2}^A \), which shall be computed in a given order \( k \), the large enough cluster \( C_l \) contains all possible subcluster \( C_s \) with two properties: (i) they have \( k \) or less bonds, (ii) they link the concerned sites \( j_1,j_2,i_1,i_2 \) among themselves [19]. Clearly, \( C_l \) depends on the order \( k \). But it depends also on the sites \( j_1,j_2,i_1,i_2 \) under study so that the notation \( C_l^{(k)} \) \((\{j_1,j_2,i_1,i_2\}) \) is appropriate. Note, that the order of the sites does not matter.

If some sites are omitted the constraints for the subclusters \( C_s \) are diminished since less sites must be linked. This implies in particular \( C_l^{(k)} \) \((\{j_1,j_2,i_1,i_2\}) \subset C_l^{(k)} \) \((\{j_1,i_1\}) \). Hence there can be a cluster \( A \) which contains \( C_l^{(k)} \) \((\{j_1,j_2,i_1,i_2\}) \) but does not contain \( C_l^{(k)} \) \((\{j_1,i_1\}) \) so that the hopping matrix element \( t_{j_1,i_1}^A \) is not the thermodynamic one, but the interaction \( t_{j_1,j_2;i_1,i_2}^A \) is without finite-size correction. So intermediate steps in the calculations (18) can display finite-size effects although the final result does not. In Refs. [2,3,8,13] we followed this strategy.

The second strategy is to compute for a given order \( k \) the net contributions of all clusters \( C \) with \( m \leq k \) bonds which link the sites under study. The advantage of this approach is that only smaller clusters need to be treated (\( \leq k \) bonds). The price to pay is an overhead in determining the net contribution. This requires to deduct from the total contribution of \( C \) the contributions of all subcluster of \( C \) with less bonds which link the points
under study. This must be done in order to avoid double counting. More details on this strategy can be found in Ref. [1].

For Hamiltonians with relatively simple topology, the second strategy is more powerful. For more complicated Hamiltonians, however, the task to implement the overhead without flaw can quickly become impracticable while the first strategy can still be used, at least up to a certain order of the perturbation.

### B. Effective observables

An effective Hamiltonian conserving the number of particles is useful to determine characteristic energies of the considered systems. But it is not sufficient to determine physical quantities which require more knowledge than the eigen-energies of the system. In particular, we aim at determining dynamic correlations such as \(\langle O(t)O(0) \rangle\). Then the mapping of the original Hamiltonian \(H\) to the effective Hamiltonian \(H_{\text{eff}}\) must be extended to a mapping of the original observable \(O\) to the effective observables \(O_{\text{eff}}\). Here we will assume that this has been achieved by an appropriate unitary transformation, for instance in a continuous fashion as described in the Introduction.

#### 1. Global structure

The structure of the observables can be described best by using the notation of second quantization. Thereby it can be denoted clearly how many particles are involved.

The most important difference compared to the Hamiltonian is that there is no particle conservation. Consequently, an observable creates and annihilates excitations, i.e. particles. Hence we define the operators

\[
O_{d,n} := \sum_{i_1 \cdots i_n, j_1 \cdots j_{n+d}} u_{j_1 \cdots j_{n+d}; i_1 \cdots i_n} e_{j_1}^\dagger \cdots e_{j_{n+d}}^\dagger e_{i_1} \cdots e_{i_n}.
\]

The local operators \(e_i\) have been described after Eq. (7). Again they shall appear normal-ordered, i.e. all creation operators are sorted to the left of the annihilation operators. The first index \(d\) indicates how many particles are created (\(d \geq 0\)) or annihilated (\(d < 0\)) by application of \(O_{d,n}\). The second index \(n \geq 0\) denotes how many particles have to be present before the operator \(O_{d,n}\) becomes active. The result of \(O_{d,n}\) acting on a state with less than \(n\) particles is zero.

In analogy to Eq. (5) the effective observables can be decomposed into partial observables like

\[
O_{\text{eff}} = \sum_{n=0}^{\infty} \sum_{d \geq -n} O_{d,n}.
\]

The additional feature in comparison to Eq. (5) is the sum over \(d\). Tab. I sketches the structure of the terms appearing in the partial observables \(O_{d,n}\)

| \(d/n\) | 0   | 1   | 2   | 3   |
|--------|-----|-----|-----|-----|
| ...   | ... | ... | ... | ... |
| -3    | 0   | 0   | 0   | e   |
| -2    | 0   | 0   | e   | e   |
| -1    | 1   | e   | e   | e   |
| 0     | 1   | e   | e   | e   |
| 1     | e   | e   | e   | e   |
| 2     | e   | e   | e   | e   |

TABLE I. List of appearing in the partial observables \(O_{d,n}\) which form together the effective observable \(O_{\text{eff}}\) according to Eq. (20). No prefactors or indices are given for clarity.

Let us assume that we computed \(O_{\text{eff}}\) by some technique, for instance by a CUT. Then the partial observables can be determined recursively by

\[
O_{d,n}\mid_{0 \to 0 + d} := O_{\text{eff}}\mid_{0 \to 0 + d} \quad (21a)
\]

\[
O_{d,1}\mid_{1 \to 1 + d} := O_{\text{eff}}\mid_{1 \to 1 + d} - O_{d,0}\mid_{1 \to 1 + d} \quad (21b)
\]

\[
O_{d,2}\mid_{2 \to 2 + d} := O_{\text{eff}}\mid_{2 \to 2 + d} - O_{d,0}\mid_{2 \to 2 + d} - O_{d,1}\mid_{2 \to 2 + d} \nonumber \quad \vdots
\]

\[
O_{d,n}\mid_{n \to n + d} := O_{\text{eff}}\mid_{n \to n + d} - \sum_{i=0}^{n-1} O_{d,i}\mid_{n \to n + d} \quad (21c)
\]

Here \(n \to n + d\) denotes the restriction of an operator to act on the \(n\)-particle subspace \(\mathcal{E}_n\) (domain) and to yield states in the \((n+d)\)-particle subspace \(\mathcal{E}_{n+d}\) (co-domain). The recursion is set-up in analogy to (9). It is again used that an operator \(O_{d,n}\) effectively vanishes if it is applied to less than \(n\) particles. Barring possible problems to define convergence, the validity of the recursion (21) for all \(d\) and \(n\) implies the decomposition (20).

As for the Hamiltonian the partial observables \(O_{d,n}\) can be viewed as the \(n\)-particle irreducible part of the particular observable. The notation in second quantization elegantly resolves the question how the observables act on clusters as was explained in the section II.A.2. Hence the definition (19) ensures cluster additivity and there exist cluster expansions for the partial observables. So they can be computed on finite clusters.

If dynamical correlations at zero temperature \(T = 0\) shall be described, the observables are applied to the ground state \(|0\rangle\) which is the particle vacuum [6]. Then only the partial observables \(O_{d,0}\) with \(d \geq 0\) matter. According to (21a) no corrections are necessary, i.e. the structure of the relevant part of the effective observable is given by

\[
O_{\text{eff}}^{T=0} = O_{0,0} + O_{1,0} + O_{2,0} + O_{3,0} + \ldots.
\]
This structure has been used so far in a number of investigations of spectral weights \[23,24\] and spectral densities \[13,14,25\]. It turned out that it is indeed sufficient to consider a restricted number of particles \[13,14,24\]. But the question how many particles are required to describe a certain physical quantity sufficiently well depends on the considered model, the chosen basis (What do we call a particle?) and the quantity under study.

At finite temperatures a certain number of particles will already be present in the system due to thermal fluctuations. Then the action of the partial observables $O_d,n$ with $n \geq 1$ will come into play as well. This constitutes an interesting route to extend the applicability of effective models, which were derived in the first place at zero temperature, to finite temperatures.

2. Computational aspects

The recursive equations for matrix elements which can be derived from (21) are very similar to those obtained for the Hamiltonian (18). We illustrate this for the matrix elements of $O_{d,n}$. Let the bare matrix elements on a cluster $A$ be

$$
\begin{align*}
    v_j^A &:= \langle j | \mathcal{O}_{\text{eff}} | 0 \rangle \\
    v_{ji,j2,i}^A &:= \langle j_1 j_2 | \mathcal{O}_{\text{eff}}^A | i \rangle \\
    &\vdots
\end{align*}
$$

From (21) we obtain the irreducible elements as

$$
\begin{align*}
    w_j^A &= v_j^A \\
    w_{ji,j2,i}^A &= v_{ji,j2,i}^A - w_j^A \delta_{j_1,i} - w_{j1}^A \delta_{j_2,i} \\
    &\vdots
\end{align*}
$$

As for the irreducible interactions the strategy is straightforward. One has to subtract from the reducible $n$-particle matrix elements $v^A$ the contributions which come from the $m$-particle irreducible matrix elements $w^A$ with $m < n$. With this strategy also other irreducible matrix elements can be determined in a straightforward manner.

So far our considerations were general in the sense that it did not matter how we achieved the mapping. Next we focus on the actual perturbative evaluation of the matrix elements on finite clusters. For simplicity, we assume as before that the perturbative part of the Hamiltonian links only nearest-neighbour sites. Let us consider for instance $w_{ji,j2,i}^A$. We assume that the observable $\mathcal{O}$ is also local, i.e. acts on a certain site only, or is a sum of such terms. If the observable is a sum of local terms then the transformation of each term separately and subsequent summation yields the result. So without loss of generality we consider $\mathcal{O}$ to affect only site $p$. Then we have to compute the matrix elements for clusters linking the four sites $j_1, j_2, i, p$. If $\mathcal{O}$ itself is a product of operators affecting several sites $p_i$ then the observable $\mathcal{O}$ itself links these sites $p_i$. Apart from this difference compared to the matrix elements of the effective Hamiltonian, we may copy the remaining steps from there:

There are again the two strategies. Either the calculation in order $k$ is performed on a cluster $C_k$ large enough so that all subclusters of $k$ bonds linking the relevant sites $j_1, j_2, i, p$ are comprised in $C_k$ \[13,14,26,27\]. Or one has to add the net contributions of all different clusters with $k$ or less bonds which link the relevant sites $j_1, j_2, i, p$ [25]. In either way the results for spectral densities can be obtained.

III. TRANSFORMATION OF THE HAMILTONIAN

So far no particular property of the transformation providing the effective operators $H_{\text{eff}}$ and $O_{\text{eff}}$ was assumed. The only prerequisites were the existence of a counting operator $Q$, which counts the number of elementary excitations, i.e. particles, and the conservation of this number of particles by $H_{\text{eff}}$: $[H_{\text{eff}}, Q] = 0$.

Here we specify a particular transformation leading to $[H_{\text{eff}}, Q] = 0$. This section is a very brief summary of Ref. [8] which is necessary to fix the ideas and the notation for the subsequent section dealing with the transformation yielding the effective observables.

For simplicity we restrict the considered systems in the following way: The problem can be formulated as perturbation problem as in Eq. (2) with the properties

(A) The unperturbed part $U$ has an equidistant spectrum bounded from below. The difference between two successive levels is the energy of a particle, i.e. $Q = U$.

(B) There is a number $N \geq N > 0$ such that the perturbing part $V$ can be split as $V = \sum_{n=-N}^{N} T_n$ where $T_n$ increments (or decrements, if $n < 0$) the number of particles by $n$: $[Q, T_n] = nT_n$.

Condition (A) allows to introduce the particularly simple and intuitive choice $Q = U$. Note that the restrictions of (A) are not too serious in practice since very often the deviations from an equidistant spectrum can be put into the perturbation $V$. Conditions (A) and (B) together imply that the starting Hamiltonian $H$ has a block-band-diagonal structure as depicted in Fig. 1. The perturbation $V$ connects states of different particle numbers only if the difference is a finite number $\leq N$. Note that very many problems in physics display this property, for a discussion of interacting fermions see Ref. [5,6]. So far, most applications consider $N = 1$ [3,28] and $N = 2$ [2,8,10,13,14,21,24,26,27,29], but calculations for higher $N$ are also possible [30].

We solve the flow equation (4) for the Hamiltonian (2) obeying the conditions (A) and (B) perturbatively, that
means up to a certain order in the expansion parameter $x$. The ansatz used is

$$H(x; \ell) = U + \sum_{k=1}^{\infty} x^k \sum_{|m| = k} F(\ell; m) T(m),$$

(25)

with unknown real functions $F(\ell; m)$ for which the flow equation (4) yields non-linear recursive differential equations [8]. The notation comprises

$$m = (m_1, m_2, m_3, \ldots, m_k)$$

with (26a)

$$m_i \in \{0, \pm 1, \pm 2, \ldots, \pm N\}$$

(26b)

$$|m| = k$$

(26c)

$$T(m) = T_{m_1} T_{m_2} T_{m_3} \cdots T_{m_k}$$

(26d)

$$M(m) = \sum_{i=1}^{N} m_i$$.

(26e)

The second sum in ansatz (25) runs over all indices $m$ of length $|m| = k$. Thereby, $H(x; \ell)$ includes all possible virtual excitation processes $T(m)$ in a given order $x^k$ multiplied by the weight $F(\ell; m)$.

The optimum choice for the infinitesimal generator $\eta$ of the unitary transformation reads

$$\eta(x; \ell) = \sum_{k=1}^{\infty} x^k \sum_{|m| = k} \text{sgn}(M(m)) F(\ell; m) T(m).$$

(27)

In the eigen-basis $|n\rangle$ of $Q$, i.e. $Q|n\rangle = n|n\rangle$, the matrix elements of the generator $\eta$ read

$$\eta_{i,j}(x; \ell) = \text{sgn}(Q_i - Q_j) H_{i,j}(x; \ell),$$

(28)

with the convention $\text{sgn}(0) = 0$. This choice keeps the the flowing Hamiltonian block-band diagonal also at intermediate values of $\ell$ [8,11]. For $\ell \to \infty$ the generator (28) eliminates all parts of $H(x; \ell)$ changing the number of particles so that $[H_{\text{eff}}, Q] = 0$ with $H_{\text{eff}} := H(\ell = \infty)$.

For the functions $F(\ell; m)$ a set of coupled differential equations is determined by inserting Eqs. (25) and (27) in the flow equation (4) and comparing coefficients. The differential equations are recursive [8]. The functions $F$ of order $k + 1$, i.e. $F(\ell; m)$ with $|m| = k + 1$, are determined by the functions $F$ of order $k$. The initial conditions are $F(0; m) = 1$ for $|m| = 1$ and $F(0; m) = 0$ for $|m| > 1$. The functions are sums of monomials with structure $(p/q)^{\ell} \exp(-2\mu \ell t)$, where $p, q, t, \mu > 0$ are integers. This allows to implement a computer-aided iterative algorithm for the computation of the functions $F$ [8].

The following symmetry relations hold

$$F(\ell; m) = F(\ell; (-m_k, \ldots, -m_1))$$

(29a)

$$F(\ell; m) = F(\ell; (-m_1, \ldots, -m_k))(-1)^{|m|+1}.$$  

(29b)

Relation (29a) reflects the hermiticity of the Hamiltonian. The block-band diagonality for all $\ell$ implies

$$F(\ell; m) = 0 \quad \text{for} \quad |M(m)| > N.$$

(30)

In the limit $\ell \to \infty$ the coefficients $C(m) := F(\ell; m)$ are obtained. They are available in paper form [8,28] and electronically [31]. The effective Hamiltonian is given by the general form

$$H_{\text{eff}}(x) = U + \sum_{k=1}^{\infty} x^k \sum_{|m| = k} C(m) T(m),$$

(31)

where $M(m) = 0$ reflects the conservation of the number of particles. The action of $H_{\text{eff}}$ can be viewed as a weighted sum of particle-number conserving virtual excitation processes each of which is encoded in a monomial $T(m)$. We want to emphasize that the effective Hamiltonian $H_{\text{eff}}$ with known coefficients $C(m)$ can be used straightforward in all perturbative problems that meet conditions (A) and (B).

![FIG. 1. Block-band diagonal Hamilton matrix for $N = 1$ in the eigen-basis $|n\rangle$ of the operator $Q$ which counts the number of particles. The unperturbed Hamiltonian $H(x = 0) = U$ and the effective Hamiltonian $H_{\text{eff}}$ have matrix elements in the dark areas only: $[H_{\text{eff}}, Q] = 0$. For non-degenerate ground state $H_{00}$ is a 1 $\times$ 1 matrix. The dimension of $H_{n,n}$ grows roughly like $L^n$ with system size $L$. The perturbation $V$ can lead to overlap matrices indicated as light boxes. The empty boxes contain vanishing matrix elements only.](image)

IV. TRANSFORMATION OF OBSERVABLES

To calculate physical quantities which do not only depend on the eigen-energies the relevant observables must be known. The conceptual simplicity of unitary transformations implies that the observables must be subject to the same unitary transformation as the Hamiltonian. In this section we describe how the perturbative CUT method can be extended to serve this purpose.

Consider the observable $O$. It is mapped according to the flow equation

$$\frac{\partial O(x; \ell)}{\partial \ell} = [\eta(x; \ell), O(x; \ell)],$$

(32)
where the same generator $\eta(x; \ell)$, given in Eq. (27), as in Eq. (4) is to be used to generate the transformation. In analogy to Eq. (25) we employ the ansatz

$$
O(x; \ell) = \sum_{k=0}^{\infty} z^k \sum_{l=1}^{k+1} G(\ell; m_l; i) O(m_l; i),
$$

(33)

where the $G(\ell; m_l; i)$ are real-valued functions for which the flow equation (32) yields recursive differential equations. The operator products $O(m_l; i)$ are given by

$$
O(m_l; i) := T_{m_1} \cdots T_{m_l-1} OT_{m_l} \cdots T_{m_k},
$$

(34)

where we use the notation of the Eqs. (26). The integer $i$ denotes the position in $O(m_l; i)$ at which the operator $O$ is inserted in the sequence of the $T_{m_l}$. The starting condition is $O(x; 0) = O(x)$ and the final result is found at $\ell = \infty$: $O_{\text{eff}}(x) := O(x; \infty)$.

Inserting the ansatz (34) for $O(x; \ell)$ and the generator $\eta(x; \ell)$ from (27) into the flow equation (32) yields

$$
\sum_{k=0}^{\infty} x^k \sum_{l=1}^{k+1} \frac{\partial}{\partial \ell} G(\ell; m_l; i) O(m_l; i) = \sum_{k_1=1}^{\infty} \sum_{k_2=0}^{\infty} x^{k_1+k_2} \sum_{|m_l| = k_1}^{k_2+1} \sum_{|m_l'| = k_2} F(\ell; m_l') G(\ell; m_l''; i) \times \operatorname{sgn}(M(m_l')) [T(m_l'), O(m_l''; i)].
$$

(35)

The functions $F(\ell; m)$ are known from the calculations described in the previous section III pertaining to the transformation of the Hamiltonian. The sums denoted by expressions of the type $|m_l| = k$ run over all multi-indices $m_l$ of length $k$.

Comparing coefficients in Eq. (35) yields a set of recursive differential equations for the functions $G(\ell; m_l; i)$. To ease the comparison of coefficients we split a specific $m_l$ with fixed in two parts as defined by $i$

$$
m_l = (m_l, m_i),
$$

(36)

with $|m_l| = i - 1$ and $|m_i| = k - i + 1$ such that the splitting reflects the structure of $O(m_l; i)$ in (34). Then the explicit recursions can be denoted by

$$
\frac{\partial}{\partial \ell} G(\ell; m_i; i) = \sum_{m_l = (m_l, m_i)} \operatorname{sgn}(M(m_l)) F(\ell; m_l) G(\ell; (m_l, m_i); i - |m_l|) - \sum_{m_l = (m_l, m_i)} \operatorname{sgn}(M(m_l)) F(\ell; m_l) G(\ell; (m_l, m_i); i).
$$

(37)

The recursive nature of these equations becomes apparent by observing that the summations $m_l = (m_l, m_i)$ and $m_i = (m_i, m_i)$ are performed over all non-trivial breakups of $m_l$ and $m_i$. For instance, the restriction $m_l = (m_1, m_2, \ldots, m_{i-1}) \vdash (m_i, m_i)$ with $m_i \neq 0$ means, that one has to sum over the breakups

$$
m_i = (m_1) \quad \text{and} \quad m_l = (m_2, \ldots, m_{i-1})
$$

$$
m_i = (m_1, m_2) \quad \text{and} \quad m_l = (m_3, \ldots, m_{i-1})
$$

$$\vdots
$$

$$m_i = (m_1, m_2, \ldots, m_{i-1}) \quad \text{and} \quad m_l = () .
$$

(38)

This implies that the $G(\ell; m_l; i)$ appearing on the right side of Eq. (37) are of order $k - 1$ or less. Once they are known the function on the left hand side of order $k$ can be computed. By iteration, all functions can be determined. The initial conditions follow from $O(x; \ell = 0) = O$ and read

$$
G(0; m_i; 1) = 1 \quad \text{for} \quad |m_l| = 0 
$$

$$
G(0; m_l; i) = 0 \quad \text{for} \quad |m_l| > 0 .
$$

(39a)

(39b)

By iteration of (37), all functions can be determined.

We briefly discuss two examples to illustrate how the Eqs. (37) work. Let us assume $N = 2$. All zero order functions $G(\ell; (1), 1)$ are equal to 1. Since there is no breakup of (), as would be required by the sums on the right hand side of Eqs. (37), the right hand sides vanish identically, whence $G(\ell; (1), 1) = 1$ for all values of $\ell$.

The first order function $G(\ell; (1), 2)$ is given by

$$
\frac{\partial}{\partial \ell} G(\ell; (1), 2) = \operatorname{sgn}[M((1))] F(\ell; (1)) \cdot G(\ell; (1))
$$

$$
e^{-\ell} \cdot 1 ,
$$

(40)

where $F(\ell; (1)) = e^{-\ell}$ is taken from Eq. (15) in Ref. [8]. With the initial condition $G(0; (1), 2) = 0$ from (39) the differential equation (40) yields

$$
G(\ell; (1), 2) = 1 - e^{-\ell} \frac{1}{\ell \rightarrow \infty} .
$$

(41)

As a second example we consider a second order function where we can use the above result

$$
\frac{\partial}{\partial \ell} G(\ell; (2), 3) = \operatorname{sgn}[M((-2, 1))] F(\ell; (-2, 1)) G(\ell; (1), 1)
$$

$$+ \operatorname{sgn}[M((-2))] F(\ell; (-2)) G(\ell; (1), 2) = - (e^{-3\ell} - e^{-\ell}) \cdot 1 \cdot e^{-2\ell} \cdot (1 - e^{-\ell})
$$

$$= e^{-\ell} - e^{-2\ell} .
$$

(42a)

(42b)

(42c)

Again the functions $F$ are taken from Eq. (15) in Ref. [8]. Integrating the result (42c) using the initial condition (39) leads to

$$
G(\ell; (-2, 1), 3) = - e^{-\ell} + \frac{1}{3} e^{-2\ell} + 1 - \frac{1}{2} \frac{1}{\ell \rightarrow \infty} .
$$

(43)
This kind of calculation carries forward to higher orders. The functions $G$ – like the functions $F$ – are sums of simple monomials $(p/q)^{\ell^i} \exp(-2\mu \ell)$, where $p, q, i, (\mu > 0)$ are integers. Thus the integrations are always straightforward

$$\int_0^\ell d\ell' \ell'^i = \frac{1}{i+1} \ell^{i+1}$$

(44a)

$$\int_0^\ell d\ell' \ell'^i e^{-2\mu \ell'} = \frac{i!}{2\mu} \left[ \frac{1}{(2\mu)^i} - e^{-2\mu \ell} \sum_{j=0}^i \frac{\ell^j}{j!(2\mu)^j} \right]$$

(44b)

and can easily be implemented in a computer-algebraic programme. The remaining implementation follows very much the same line as described previously for the functions $F$ [8].

In analogy to Eqs. (29) for $F$ two symmetry relations hold for $G$. With \( \vec{m} = (m_1, \ldots, m_k) \) they read

$$G(\ell; \vec{m}; i) = G(\ell; (-m_k, \ldots, -m_1); k - i + 2)$$

(45a)

$$G(\ell; \vec{m}; i) = G(\ell; (-m_1, \ldots, -m_k); i)(-1)^{|\vec{m}|}$$

(45b)

as can be shown by induction. The first symmetry (45a) holds if $\mathcal{O}$ is hermitian. Unfortunately, there is no equivalence to Eq. (30) so that a possible initial block-band structure in $\mathcal{O}(x; 0)$ is generically lost in the course of the transformation, i.e. for $\ell > 0$.

In the limit $\ell \to \infty$ the coefficients $\tilde{C}(\vec{m}; i) := G(\infty; \vec{m}; i) \in \mathbb{Q}$ are obtained as rational numbers. So we retrieve finally

$$\mathcal{O}_{\text{eff}}(x) = \sum_{k=0}^{\infty} x^k \sum_{i=1}^{k+1} \tilde{C}(\vec{m}; i) \mathcal{O}(\vec{m}; i)$$

(46)

similar to Eq. (31). We will make the coefficients $\tilde{C}(\vec{m}; i)$ available electronically [31]. Note that $\mathcal{O}_{\text{eff}}$ is not a particle-conserving quantity as is obvious from the fact that the sum over $|\vec{m}|$ is not restricted to $M(\vec{m}) = 0$. In order to see the net effect of $\mathcal{O}_{\text{eff}}(x)$ on the number of particles explicitly it is helpful to split the bare operator accordingly $\mathcal{O} = \sum_{n=0}^{N} T_n$, where $T_n$ increments (or decrements, if $n < 0$) the number of particles by $n$: $[Q, T_n] = n T_n'$. The difference between the bare initial observable $\mathcal{O}$ and the representation (46) must be viewed as vertex correction which comes into play since the bare initial excitations are not the true eigen-excitations of the interacting system. We like to stress that the formalism presented introduces the notions of $n$-particle irreducibility, vertex correction and so on without starting from the limit of non-interacting conventional particles such as bosons or fermions.

V. CONCLUSIONS

A. Summary

In this article we have presented an approach to calculate energies and observables for quantum multi-particle systems defined on lattices. The article has two main parts. In the first part (Sect. II), we assumed the existence of a mapping of the original problem to an effective one in which the number of elementary excitations, the so-called (quasi-)particles, is conserved. The general structure of the effective Hamiltonians and the observables is analysed. We found that a classification of the various contributions in terms of the number of particles concerned is most advantageous. To this end we introduced a notation in second quantization which does not, however, require non-interacting fermions or bosons. Generically, hard-core bosons are involved.

We found the formulation in second quantization particularly intuitive. It provides in a natural way the irreducible quantities on the operator level which display cluster additivity. We like to emphasize that the definition of irreducible operators is not a trivial task if a strong-coupling situation is considered as was done in the present paper. No limit of non-interacting bosons or fermions is assumed. Since the definition of irreducible operators is completely general it allows to compute the $n$-particle contribution for arbitrary $n$. For instance the formulae for the 3-particle interactions are given for the first time in the literature.

The irreducible interactions and vertex corrections possess a cluster expansion so that they can be computed on finite clusters provided that the Hamiltonian is of finite range. This property is the basis for the real-space treatment of many spin systems.

In the second part (Sects. III and IV), we described an actual mapping which provides effective operators. The mapping is based on continuous unitary transformations. In this paper we constructed the mapping perturbatively (see 'Outlook'). In Sect. III the treatment of the Hamiltonian is given. The computation of the effective Hamiltonian requires the solution of a set of recursive non-linear differential equations. For the perturbative set-up under study these equations can be solved in full generality, i.e. no particular details of the model must be known.

In Sect. IV we have given the calculational steps to compute effective observables. Again recursive differential equations have to be solved. But they are linear since the transformation of the Hamiltonian is known. For the perturbative set-up under study also the equations for the observables can be solved in full generality, i.e. no particular details of the model must be known.

The above approach has been used to compute spectral functions, i.e. dynamical correlations, in a number of models [2, 3, 8, 10, 13, 14, 21, 24, 26–30]. These results may serve as examples for the utility of the approach presented.
We like to point out two important consequences of the formulation of the effective operators in second quantization. Both implications are based on the observation that the irreducible operators are defined on the whole Hilbert space, i.e. not only for a small number of particles. The matrix elements of the $n$-particle irreducible operators can be computed considering only $n$-particles. But the resulting operators hold for arbitrary number of particles.

a. Consequence 1: The effective Hamiltonian is valid at finite temperatures. Hence it is possible to extend the results obtained in the first place at zero temperature to finite temperatures. The technical difficulty arising is to treat the interactions properly, in particular the hard-core constraint. But the description in terms of effective particles helps to tackle this situation. Let us recall that at zero temperature no excitation, i.e. no particle, is present. At low temperatures only a small density of particles will be in the system. So it is well justified to use a ladder approximation. This approximation is also suited to deal with the hard-core constraint (Brückner approach) [32,33]. Note that the problems linked to the existence of anomalous Green functions [33] do not occur if the particle-conserving, effective Hamiltonian is used. Thus the Brückner approach for the effective Hamiltonian after a suitable mapping [4,8] is well justified and represents a very promising route to treat finite temperatures.

b. Consequence 2: So far the mapping to an effective model has been constructed perturbatively. That means that all operators, the Hamiltonian $H$, the generator $\eta$ and the observables $O_i$ are given in a series of some small parameter $x$. In actual applications these series are suitably extrapolated. But a certain caveat persists if the starting point is a local Hamiltonian. Then a calculation up to a certain order describes processes of a certain finite range only. This restriction can be partly overcome by extrapolating in momentum space, e.g. for dispersion relations $\omega(k)$. But it is difficult to extrapolate the matrix elements of the 2-particle irreducible interaction because it is not diagonal in all momenta.

This problem can be overcome by performing the continuous unitary transformation directly on the level of the $n$-particle irreducible operators. An ansatz for the effective Hamiltonian is chosen comprising for instance all possible irreducible $n$-particle terms and similar terms creating and annihilating particles. This ansatz is inserted in the flow equation (4). Comparison of the coefficients $t_{j_1,\ldots,j_i}$ and $\partial t_{j_1,\ldots,j_i}$ in front of the terms $e_{j_1}^\dagger \cdots e_{j_i}^\dagger$ yields coupled non-linear differential equations. These differential equations represent renormalization equations for the problem under study. We call this type of transformation a self-similar one since the kind of terms retained stays the same. Again, the formulation in second quantization allows a significant generalization.

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APPENDIX A: THREE-PARTICLE IRREDUCIBLE INTERACTION

Here we complete the formulae for the irreducible 3-particle interaction which was given in Eq. (18). The corrections $A_0$, $A_1$ and $A_2$ result from $H_0$, $H_1$ and $H_2$, respectively, as given in (9). They read

$$A_0 = E_0^A \left[ \delta_{j_1,i_1} \delta_{j_2,i_2} \delta_{j_3,i_3} + \delta_{j_1,i_2} \delta_{j_2,i_3} \delta_{j_3,i_1} + \delta_{j_1,i_3} \delta_{j_2,i_1} \delta_{j_3,i_2} \right]$$  \hspace{1cm} (A1a)

$$A_1 = \delta_{j_1,i_1} t_{j_2}^A \delta_{j_3,i_2} + \delta_{j_1,i_2} \delta_{j_2,i_1} t_{j_3}^A + \delta_{j_1,i_3} \delta_{j_2,i_2} t_{j_3}^A + \delta_{j_1,i_2} \delta_{j_2,i_3} t_{j_1}^A + \delta_{j_1,i_3} \delta_{j_2,i_1} t_{j_3}^A + \delta_{j_1,i_1} \delta_{j_2,i_3} t_{j_2}^A + \delta_{j_1,i_3} \delta_{j_2,i_2} t_{j_1}^A + \delta_{j_1,i_2} \delta_{j_2,i_1} t_{j_3}^A$$  \hspace{1cm} (A1b)

$$A_2 = \delta_{j_1,i_1} \delta_{j_2,i_2} \delta_{j_3,i_3} + \delta_{j_1,i_2} \delta_{j_3,i_1} \delta_{j_2,i_3} + \delta_{j_1,i_3} \delta_{j_2,i_2} \delta_{j_3,i_1} + \delta_{j_1,i_3} \delta_{j_2,i_1} \delta_{j_3,i_2} + \delta_{j_1,i_1} \delta_{j_3,i_2} \delta_{j_2,i_3} + \delta_{j_1,i_2} \delta_{j_3,i_1} \delta_{j_2,i_3} + \delta_{j_1,i_3} \delta_{j_2,i_1} \delta_{j_3,i_2} + \delta_{j_1,i_2} \delta_{j_3,i_1} \delta_{j_2,i_3}$$  \hspace{1cm} (A1c)

where we used the shorthands

$$\delta_{j_1,j_2,i_1,i_2} := \delta_{j_1,i_1} \delta_{j_2,i_2} + \delta_{j_1,i_2} \delta_{j_2,i_1}$$  \hspace{1cm} (A2a)

$$t_{j_2}^A := t_{j_1,j_2,i_1,i_2} + t_{j_1,j_2,i_1} + t_{j_1,j_2,i_2} + t_{j_2,j_1,i_1,i_2}$$  \hspace{1cm} (A2b)

While the actual formulae are lengthy the underlying principle is straightforward (see main text). Note that in concrete realizations it is often advantageous to denote only one representative of the states which do not
change on interchange of particles ($|ji⟩ = |ij⟩$). Furthermore, certain problems allow to exploit higher particular symmetries like spin rotation symmetry. Then additional permutation symmetries among the various quantum numbers constituting the multi-index can be exploited leading to the appearance of exchange-parity factors.

[1] M. P. Gelfand and R. R. P. Singh, Adv. Phys. 49, 93 (2000).
[2] G. S. Uhrig and B. Normand, Phys. Rev. B 58, R14705 (1998).
[3] C. Knetter, A. Bührer, E. Müller-Hartmann, and G. S. Uhrig, Phys. Rev. Lett. 85, 3958 (2000).
[4] S. Trebst et al., Phys. Rev. Lett. 85, 4373 (2000).
[5] C. P. Heidbrink and G. S. Uhrig, Phys. Rev. Lett. 88, 146401 (2002).
[6] C. P. Heidbrink and G. S. Uhrig, Eur. Phys. J. B 30, 443 (2002).
[7] S. R. White, J. Chem. Phys. 117, 7472 (2002).
[8] C. Knetter and G. S. Uhrig, Eur. Phys. J. B 13, 209 (2000).
[9] F. J. Wegner, Ann. Physik 3, 77 (1994).
[10] J. Stein, J. Stat. Phys. 88, 487 (1997).
[11] A. Mielke, Eur. Phys. J. B 5, 605 (1998).
[12] S. K. Kehrein and A. Mielke, Ann. Physik 6, 90 (1997).
[13] C. Knetter, K. P. Schmidt, M. Grüninger, and G. S. Uhrig, Phys. Rev. Lett. 87, 167204 (2001).
[14] K. P. Schmidt, C. Knetter, and G. S. Uhrig, Europhys. Lett. 56, 877 (2001).
[15] W. Zheng et al., Phys. Rev. B 63, 144410 (2001).
[16] Another way to deal with the ambiguity would be to introduce a certain ordering among the indices. Then only one representative of the two (or more) identical states needs to be kept [3,13].
[17] M. P. Gelfand, R. R. P. Singh, and D. A. Huse, J. Stat. Phys. 59, 1093 (1990).
[18] M. P. Gelfand, Solid State Commun. 98, 11 (1996).
[19] Depending on the details of the interaction on the bonds it may be sufficient to consider smaller clusters than mentioned in the main text, for instance a pure nearest-neighbour spin exchange reduces the range of virtual excursions. Frustration is another mechanism which reduces the range of the effective processes, see e.g. the Shastry-Sutherland model [3,20,21].
[20] S. Miyahara and K. Ueda, Phys. Rev. Lett. 82, 3701, (1999).
[21] E. Müller-Hartmann, R. R. P. Singh, C. Knetter, and G. S. Uhrig, Phys. Rev. Lett. 84, 1808 (2000).
[22] W. Zheng et al., Phys. Rev. B 63, 144411 (2001).
[23] R. R. P. Singh and Z. Weihong, Phys. Rev. B 59, 9911 (1999).
[24] K. P. Schmidt and G. S. Uhrig, cond-mat/0211627.
[25] W. Zheng, C. J. Hamer, and R. R. P. Singh, cond-mat/0211346.