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Abstract
For many-particle systems defined on lattices we investigate the global structure of effective Hamiltonians and observables obtained by means of a suitable basis transformation. We study transformations which lead to effective Hamiltonians conserving the number of excitations. The *same* transformation must be used to obtain effective observables. The analysis of the structure shows that effective operators give rise to a simple and intuitive perspective on the initial problem. The systematic calculation of n-particle irreducible quantities becomes possible constituting a significant progress. Details on how to implement the approach perturbatively for a large class of systems are presented.

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1. Introduction

Effective models are at the very centre of theoretical physics since they allow us to focus on the essential physics of a problem without being distracted by unnecessary complexity. Hence it is very important to make use of *systematic* means to derive effective models. Here we will present the mathematical structure of a certain kind of effective model, 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 paper is the perturbative computation of effective Hamiltonians and observables. Such computations are a standard technique for ground-state energies (zero-particle terms) and dispersion relations (one-particle terms) (see [1] and references therein). But the possibility of computing 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 paper, consists in the non-perturbative, renormalizing realization of the transformation of the initial model to the effective model which conserves the number of particles. Examples of this approach are realized in fermionic models [5–7].

1.1. Starting point

We consider models which are defined on a lattice Γ. 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_ν acting on a *finite* number of sites in the vicinity of the site ν,

$$H = \sum_{\nu \in \Gamma} h_\nu. \tag{1}$$

We further assume that H can be split as

$$H(x) = U + xV \tag{2}$$

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 $0 \leqslant x \leqslant x_c$ 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 paper, we advocate using a continuous unitary transformation (CUT) [8–11] in order to achieve a systematically controlled mapping of the kind described above which leads to

$$[H_{\text{eff}}, Q] = 0 \tag{3}$$

i.e. H_{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 $\mathcal{O}_{\text{eff}}$ from the original observables $\mathcal{O}$.

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]

$$\partial_\ell H = [\eta(\ell), H(\ell)] \tag{4}$$

where $l \in [0, \infty]$ 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 η of the transformation it can be designed such that it 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 would 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 methods other 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].

1.2. Set-up

In section 2 we analyse global structural aspects of effective operators. The basic prerequisite will be equation (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.

Section 3 is a preparatory section in which the perturbative CUT for Hamilton operators of a certain kind is constructed. Low-dimensional spin models on lattices are among the models which can be treated in this way.

Section 4 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 us to compute the experimentally relevant spectral functions. So the extension from Hamiltonians to observables is an important one.

The paper is concluded in section 5.

2. The structure of effective operators

In this section, we *assume* that we are able to construct a mapping such that H_{eff} fulfils equation (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_{eff} and $\mathcal{O}_{\text{eff}}$ are polynomials in x.

2.1. The effective Hamiltonian

2.1.1. Global structure.   We will show that H_{eff} can be written as

$$H_{\text{eff}} = H_0 + H_1 + H_2 + H_3 + \cdots \tag{5}$$

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.

Equation (5) comprises already a route to determine the properties of H_{eff} in a sequence of approximate treatments. The very first step is to know the ground-state energy 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 equation (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,

$$
\begin{array}{ll}
|0\rangle & \text{ground state (particle vacuum)} \\
|i\rangle & \text{state with one particle on site } i \\
|i_1 i_2\rangle & \text{state with two particles on sites } i_1 \text{ and } i_2 \\
\vdots &
\end{array}
\tag{6}
$$

i.e. $Q|0\rangle = 0|0\rangle$, $Q|i\rangle = 1|i\rangle$ and $Q|ij\rangle = 2|ij\rangle$ and so on. These states span the global Hilbert space $\mathcal{E}$ of the physical system under study. Dealing with (hard-core) bosons $|i_1 i_2\rangle$ and $|i_2 i_1\rangle$ are identical states. This indistinguishability causes a certain ambiguity. This ambiguity can be remedied for instance by assuming that coefficients depending on several indices $i_1 i_2 \ldots i_n$ are even under permutation of any pair of these indices[1]. 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 $\mathcal{R}|_n$ 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

$$H_0 := E_0 \mathbf{1} \tag{7a}$$

$$H_1 := \sum_{i;j} t_{j;i} e_j^\dagger e_i \tag{7b}$$

$$H_2 := \sum_{i_1 i_2; j_1 j_2} t_{j_1 j_2; i_1 i_2} e_{j_1}^\dagger e_{j_2}^\dagger e_{i_2} e_{i_1} \tag{7c}$$

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[1] 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].

$$\vdots$$

$$H_n := \sum_{i_1...i_n;\,j_1...j_n} t_{j_1...j_n;i_n...i_1} e^{\dagger}_{j_1} \ldots e^{\dagger}_{j_n} e_{i_n} \ldots e_{i_1} \tag{7d}$$

where $\mathbf{1}$ 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 a 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 $\mathbf{i}$ and $\mathbf{j}$.

As an example let us consider that there are three kinds of particles per site, 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 $\mathbf{i} = (i, \alpha)$, where i denotes the site and α 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 $e^{\dagger}_{i,\alpha}$ are the 4×4 matrices

$$e^{\dagger}_{i,-1} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \tag{8a}$$

$$e^{\dagger}_{i,0} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \tag{8b}$$

$$e^{\dagger}_{i,1} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}. \tag{8c}$$

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 3×3 block can be viewed as combined annihilation and creation processes: the matrix $M_{\alpha,\beta}$ with all elements zero except the one at (α, β) corresponds to the process $e^{\dagger}_{i,\alpha} e_{i,\beta}$. A finite matrix element in the upper left 1×1 block, i.e. the singlet–singlet channel, can be expressed in normal-ordered fashion as $\mathbf{1}_4 - \sum_\alpha e^{\dagger}_{i,\alpha} e_{i,\alpha}$. 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 equations (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 $H_n|_m$ vanishes for $m < n$. This follows directly from the normal ordering of

the creation and annihilation operators in equation (7). Then we can proceed iteratively by requiring that H_{eff} applied to n particles corresponds to $H_0 + H_1 + \cdots + H_n$ (n arbitrary but fixed). Solving for H_n yields the recursions

$$H_0|_0 := H_{\text{eff}}|_0 \tag{9a}$$

$$H_1|_1 := H_{\text{eff}}|_1 - H_0|_1 \tag{9b}$$

$$H_2|_2 := H_{\text{eff}}|_2 - H_0|_2 - H_1|_2 \tag{9c}$$

$$\vdots$$

$$H_n|_n := H_{\text{eff}}|_n - \sum_{i=0}^{n-1} H_i|_n. \tag{9d}$$

Assuming that H_{eff} is calculated beforehand one starts evaluating E_0 by means of the first definition. The result entirely defines H_0. The restriction $H_0|_1$ is then used in the second equation to extract the $t_{j;i}$ 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 equation (9d) holds for any number of particles and since $H_n|_m$ vanishes for $m < n$ we obtain equation (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 equation (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 particle counted by some operator Q.

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

2.1.2. Cluster additivity. Here we focus on formal aspects of a perturbative approach generalizing results obtained previously for zero-particle properties [16] and for one-particle properties [17]. The feature that the Hamiltonian is of finite range on the lattice is exploited. Then equations (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 $\mathcal{R}^C$ we denote an operator which acts only on the Hilbert space $\mathcal{E}^C$ of C. If $\bar{C}$ 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 $\mathcal{E} = \mathcal{E}^C \otimes \mathcal{E}^{\bar{C}}$ by

$$\mathcal{R} := \mathcal{R}^C \otimes \mathbf{1}^{\bar{C}}. \tag{10}$$

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* iff it can be decomposed as

$$\mathcal{R}^C = \mathcal{R}^A \otimes \mathbf{1}^B + \mathbf{1}^A \otimes \mathcal{R}^B. \tag{11}$$

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

The cluster additivity of H_{eff}^C is obvious since A and B are assumed to be disconnected. So they can be viewed as physically independent systems. Hence

$$H_{\text{eff}}^C = H_{\text{eff}}^A \otimes \mathbf{1}^B + \mathbf{1}^A \otimes H_{\text{eff}}^B. \tag{12}$$

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

$$H_n^C = H_n^A \otimes \mathbf{1}^B + \mathbf{1}^A \otimes H_n^B \tag{13}$$

fulfil the recursion (9) for the operators defined for the cluster C. Hence the operators H_{eff} and H_n are indeed cluster additive.

It is instructive to see that $H_{\text{eff}}|_n$ is *not* cluster additive, contrary to what one might have thought. Let us consider the tentative identity

$$H_{\text{eff}}^C\big|_n = H_{\text{eff}}^A\big|_n \otimes \mathbf{1}^B + \mathbf{1}^A \otimes H_{\text{eff}}^B\big|_n. \tag{14}$$

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 $\mathbf{1}^A$ and $\mathbf{1}^B$ are applied is not fixed. So no cluster additivity is given for the $H_{\text{eff}}|_n$.

The fact that cluster additivity holds only for particular quantities was noted previously for $n = 1$ [17]. For $n = 2$, the subtraction procedure was first applied in the calculations in [2] (though not given in detail). In [3, 4, 15, 20] the subtractions necessary to obtain the irreducible two-particle interaction were given in more detail. The general formalism presented in this paper 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 $e_i^\dagger$ can be used independent of the cluster in which the site i is embedded. In particular, one identifies automatically $e_i^{\dagger,C}$ with $e_i^{\dagger,A} \otimes \mathbf{1}^B$ if $i \in A$ and with $\mathbf{1}^A \otimes e_i^{\dagger,B}$ if $i \in B$. Hence cluster additivity is reduced to trivial statements of the kind that

$$H_1^A = \sum_{i,j \in A} t_{j;i} e_j^\dagger e_i \tag{15a}$$

$$H_1^B = \sum_{i,j \in B} t_{j;i} e_j^\dagger e_i \tag{15b}$$

implies

$$H_1^C = \sum_{i,j \in C} t_{j;i} e_j^\dagger e_i \tag{16a}$$

$$= \sum_{i,j \in A} t_{j;i} e_j^\dagger e_i + \sum_{i,j \in B} t_{j;i} e_j^\dagger e_i \tag{16b}$$

$$= H_1^A \otimes \mathbf{1}^B + \mathbf{1}^A \otimes H_1^B. \tag{16c}$$

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

Following Gelfand and co-workers [1, 16, 17] we conclude that the cluster additive quantities possess a cluster expansion. Hence all the irreducible matrix elements $t_{j;i}$ possess a cluster expansion and can be computed on finite clusters.

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

$$E_0^A := \langle 0|H_{\text{eff}}^A|0\rangle \tag{17a}$$

$$a_{j;i}^A := \langle j|H_{\text{eff}}^A|i\rangle \tag{17b}$$

$$a_{j_1 j_2; i_1 i_2}^A := \langle j_1 j_2|H_{\text{eff}}^A|i_1 i_2\rangle \tag{17c}$$

$$\vdots$$

where the indices i, j, ... may be multi-indices from now on. Put differently, E_0^A is the matrix element of $H_{\text{eff}}^A\big|_0$, the $a_{j;i}^A$ are the matrix elements of $H_{\text{eff}}^A\big|_1$, the $a_{j_1 j_2; i_1 i_2}^A$ those of $H_{\text{eff}}^A\big|_2$ and so on. The number E_0^A is the ground-state energy of cluster A. The recursive definitions (9) imply

$$t_{j;i}^A = a_{j;i}^A - E_0^A \delta_{ji} \tag{18a}$$

$$t_{j_1 j_2; i_1 i_2}^A = a_{j_1 j_2; i_1 i_2}^A - E_0^A \delta_{j_1 i_1}\delta_{j_2 i_2} - E_0^A \delta_{j_1 i_2}\delta_{j_2 i_1} - t_{j_2; i_2}^A \delta_{j_1 i_1} - t_{j_1; i_2}^A \delta_{j_2 i_1} - t_{j_2; i_1}^A \delta_{j_1 i_2} - t_{j_1; i_1}^A \delta_{j_2 i_2} \tag{18b}$$

$$t_{j_1 j_2 j_3; i_1 i_2 i_3}^A = a_{j_1 j_2 j_3; i_1 i_2 i_3}^A - A_0 - A_1 - A_2 \tag{18c}$$

$$\vdots$$

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 subclusters 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[2]. Clearly, C_l depends on the order k. But it depends also on the sites j_1, j_2, i_1, i_2

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[2] 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, 18, 19].

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 $t_{j_1;i_i}^A$ 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 [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 $m \leqslant k$ bonds which link the sites under study. The advantage of this approach is that only smaller clusters need to be treated ($\leqslant k$ 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 subclusters of C with fewer 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 [1].

For Hamiltonians with relatively simple topology, the second strategy is more powerful. For more complicated Hamiltonians, however, the task of implementing 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.

2.2. 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 $\langle \mathcal{O}(t)\mathcal{O}(0)\rangle$. Then the mapping of the original Hamiltonian H to the effective Hamiltonian H_{eff} must be extended to a mapping of the original observable $\mathcal{O}$ to the effective observables $\mathcal{O}_{\text{eff}}$. 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.

2.2.1. 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. Generically an observable creates and annihilates excitations, i.e. particles. Hence we define the operators

$$\mathcal{O}_{d,n} := \sum_{i_1 \cdots i_n; j_1 \cdots j_{n+d}} w_{j_1 \cdots j_{n+d}; i_1 \cdots i_n} e_{j_1}^\dagger \cdots e_{j_{n+d}}^\dagger e_{i_n} \cdots e_{i_1}. \tag{19}$$

The local operators e_i have been described after equation (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 ($d \geqslant 0$) or annihilated ($d < 0$) by application of $\mathcal{O}_{d,n}$. The second index $n \geqslant 0$ denotes how many particles have to be present before the operator $\mathcal{O}_{d,n}$ becomes active. The result of $\mathcal{O}_{d,n}$ acting on a state with less than n particles is zero.

Table 1. List of terms appearing in the partial observables $\mathcal{O}_{d,n}$ which form together the effective observable $\mathcal{O}_{\text{eff}}$ according to equation (20). No prefactors or indices are given for clarity.

			n	
d	0	1	2	3
...	...	...	...	...
-3	0	0	0	eee
-2	0	0	ee	$e^\dagger eee$
-1	0	e	$e^\dagger ee$	$e^\dagger e^\dagger eee$
0	1	$e^\dagger e$	$e^\dagger e^\dagger ee$	$e^\dagger e^\dagger e^\dagger eee$
1	$e^\dagger$	$e^\dagger e^\dagger e$	$e^\dagger e^\dagger e^\dagger ee$	$e^\dagger e^\dagger e^\dagger e^\dagger eee$
2	$e^\dagger e^\dagger$	$e^\dagger e^\dagger e^\dagger e$	$e^\dagger e^\dagger e^\dagger e^\dagger ee$	$e^\dagger e^\dagger e^\dagger e^\dagger e^\dagger eee$
...	...	...	...	...

In analogy with equation (5) the effective observables can be decomposed into partial observables like

$$\mathcal{O}_{\text{eff}} = \sum_{n=0}^{\infty} \sum_{d \geqslant -n} \mathcal{O}_{d,n}. \tag{20}$$

The additional feature in comparison to equation (5) is the sum over d. Table 1 sketches the structure of the terms appearing in the partial observables $\mathcal{O}_{d,n}$.

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

$$\mathcal{O}_{d,0}|_{0 \to 0+d} := \mathcal{O}_{\text{eff}}|_{0 \to 0+d} \tag{21a}$$

$$\mathcal{O}_{d,1}|_{1 \to 1+d} := \mathcal{O}_{\text{eff}}|_{1 \to 1+d} - \mathcal{O}_{d,0}|_{1 \to 1+d} \tag{21b}$$

$$\mathcal{O}_{d,2}|_{2 \to 2+d} := \mathcal{O}_{\text{eff}}|_{2 \to 2+d} - \mathcal{O}_{d,0}|_{2 \to 2+d} - \mathcal{O}_{d,1}|_{2 \to 2+d}$$

$$\vdots$$

$$\mathcal{O}_{d,n}|_{n \to n+d} := \mathcal{O}_{\text{eff}}|_{n \to n+d} - \sum_{i=0}^{n-1} \mathcal{O}_{d,i}|_{n \to n+d}. \tag{21c}$$

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 with (9). It is again used that an operator $\mathcal{O}_{d,n}$ effectively vanishes if it is applied to *fewer* 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 $\mathcal{O}_{d,n}$ 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 section 2.1.2. Hence 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 $\mathcal{O}_{d,0}$ with $d \geqslant 0$ matter. According to (21a) no corrections are necessary, i.e. the structure of the relevant part of the effective observable is given by

$$\mathcal{O}_{\text{eff}}^{T=0} = \mathcal{O}_{0,0} + \mathcal{O}_{1,0} + \mathcal{O}_{2,0} + \mathcal{O}_{3,0} + \cdots. \tag{22}$$

This structure has been used so far in a number of investigations of spectral weights [21, 22] and spectral densities [13, 14, 23]. It turned out that it is indeed sufficient to consider a restricted number of particles [13, 14, 22]. 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 $\mathcal{O}_{d,n}$ with $n \geqslant 1$ 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.

2.2.2. 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 $\mathcal{O}_{1,n}$. Let the bare matrix elements on a cluster A be

$$v_j^A := \langle j | \mathcal{O}_{\text{eff}}^A | 0 \rangle \tag{23a}$$

$$v_{j_1 j_2; i}^A := \langle j_1 j_2 | \mathcal{O}_{\text{eff}}^A | i \rangle \tag{23b}$$
$$\vdots$$

From (21) we obtain the irreducible elements as

$$w_j^A = v_j^A \tag{24a}$$

$$w_{j_1 j_2; i}^A := v_{j_1 j_2; i}^A - w_{j_1}^A \delta_{j_2 i} - w_{j_2}^A \delta_{j_1 i} \tag{24b}$$
$$\vdots$$

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 other irreducible matrix elements can also 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 $w_{j_1 j_2; i}^A$. 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 two strategies. Either the calculation in order k is performed on a cluster C_l large enough so that all subclusters of k bonds linking the relevant sites j_1, j_2, i, p are comprised in C_l [13, 14, 24, 25]. Or one has to add the *net* contributions of all different clusters with k or fewer bonds which link the relevant sites j_1, j_2, i, p [23]. In either way the results for spectral densities can be obtained.

Figure 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_{eff} have matrix elements in the dark areas only: $[H_{\text{eff}}, Q] = 0$. For the non-degenerate ground state H_{00} is a 1×1 matrix. The dimension of H_{nn} 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.

3. Transformation of the Hamiltonian

So far no particular property of the transformation providing the effective operators H_{eff} and $\mathcal{O}_{\text{eff}}$ 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_{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 [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 a perturbation problem as in equation (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 $\mathbb{N} \ni N > 0$ 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 us 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 figure 1. The perturbation V connects states of different particle numbers only if the difference is a finite number $\leqslant N$. Note that very many problems in physics display this property, for a discussion of interacting fermions see [5, 6]. So far, most applications consider $N = 1$ [3, 26] and $N = 2$ [2, 8, 10, 13, 14, 19, 22, 24, 25, 27], but calculations for higher N are also possible [28].

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

$$H(x; \ell) = U + \sum_{k=1}^{\infty} x^k \sum_{|\underline{m}|=k} F(\ell; \underline{m}) T(\underline{m}) \tag{25}$$

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

$$\underline{m} = (m_1, m_2, m_3, \ldots, m_k) \qquad \text{with} \tag{26a}$$

$$m_i \in \{0, \pm 1, \pm 2, \ldots, \pm N\} \tag{26b}$$

$$|\underline{m}| = k \tag{26c}$$

$$T(\underline{m}) = T_{m_1} T_{m_2} T_{m_3} \cdots T_{m_k} \tag{26d}$$

$$M(\underline{m}) = \sum_{i=1}^{k} m_i. \tag{26e}$$

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

The optimum choice for the infinitesimal generator η of the unitary transformation reads

$$\eta(x; \ell) = \sum_{k=1}^{\infty} x^k \sum_{|\underline{m}|=k} \text{sgn}(M(\underline{m})) F(\ell; \underline{m}) T(\underline{m}). \tag{27}$$

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

$$\eta_{i,j}(x; \ell) = \text{sgn}(Q_i - Q_j) H_{i,j}(x; \ell) \tag{28}$$

with the convention $\text{sgn}(0) = 0$. This choice keeps the flowing Hamiltonian block-band diagonal also at intermediate values of ℓ [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 $F(\ell; \underline{m})$ a set of coupled differential equations is determined by inserting equations (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. $F(\ell; \underline{m})$ with $|\underline{m}| = k + 1$, are determined by the functions F of order k. The initial conditions are $F(0; \underline{m}) = 1$ for $|\underline{m}| = 1$ and $F(0; \underline{m}) = 0$ for $|\underline{m}| > 1$. The functions are sums of monomials with structure $(p/q)\ell^i \exp(-2\mu\ell)$, where p, q, i ($\mu > 0$) are integers. This allows us to implement a computer-aided iterative algorithm for the computation of the functions F [8].

The following symmetry relations hold

$$F(\ell; \underline{m}) = F(\ell; (-m_k, \ldots, -m_1)) \tag{29a}$$

$$F(\ell; \underline{m}) = F(\ell; (-m_1, \ldots, -m_k))(-1)^{|\underline{m}|+1}. \tag{29b}$$

Relation (29a) reflects the Hermiticity of the Hamiltonian. The block-band diagonality for all ℓ implies

$$F(\ell; \underline{m}) = 0 \qquad \text{for} \quad |M(\underline{m})| > N. \tag{30}$$

In the limit $\ell \to \infty$ the coefficients $C(\underline{m}) := F(\infty; \underline{m})$ are obtained. They are available in paper form [8, 26] and electronically[3]. The effective Hamiltonian is given by the general form

$$H_{\text{eff}}(x) = U + \sum_{k=1}^{\infty} x^k \sum_{\substack{|\underline{m}|=k \\ M(\underline{m})=0}} C(\underline{m}) T(\underline{m}) \tag{31}$$

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

4. Transformation of observables

To calculate physical quantities which do not only depend on the eigen-energies the relevant observables must also 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 $\mathcal{O}$. It is mapped according to the flow equation

$$\frac{\partial \mathcal{O}(x; \ell)}{\partial \ell} = [\eta(x; \ell), \mathcal{O}(x; \ell)] \tag{32}$$

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

$$\mathcal{O}(x; \ell) = \sum_{k=0}^{\infty} x^k \sum_{i=1}^{k+1} \sum_{|\underline{m}|=k} G(\ell; \underline{m}; i) \mathcal{O}(\underline{m}; i) \tag{33}$$

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

$$\mathcal{O}(\underline{m}; i) := T_{m_1} \cdots T_{m_{i-1}} \mathcal{O} T_{m_i} \cdots T_{m_k} \tag{34}$$

where we use the notation of equations (26). The integer i denotes the position in $\mathcal{O}(\underline{m}, i)$ at which the operator $\mathcal{O}$ is inserted into the sequence of the T_m. The starting condition is $\mathcal{O}(x; 0) = \mathcal{O}(x)$ and the final result is found at $\ell = \infty$: $\mathcal{O}_{\text{eff}}(x) := \mathcal{O}(x; \infty)$.

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

$$\sum_{k=0}^{\infty} x^k \sum_{|\underline{m}|=k} \sum_{i=1}^{k+1} \frac{\partial}{\partial \ell} G(\ell; \underline{m}; i) \mathcal{O}(\underline{m}; i) = \sum_{k_1=1}^{\infty} \sum_{k_2=0}^{\infty} x^{k_1+k_2} \sum_{\substack{|\underline{m}'|=k_1 \\ |\underline{m}''|=k_2}} \sum_{i=1}^{k_2+1} F(\ell; \underline{m}') G(\ell; \underline{m}''; i)$$

$$\times \operatorname{sgn}(M(\underline{m}'))[T(\underline{m}'), \mathcal{O}(\underline{m}''; i)]. \tag{35}$$

The functions $F(\ell; \underline{m})$ are known from the calculations described in section 3 pertaining to the transformation of the Hamiltonian. The sums denoted by expressions of the type $|\underline{m}| = k$ run over all multi-indices $\underline{m}$ of length k.

---

[3] The coefficients $C(\underline{m})$ and $\tilde{C}(\underline{m})$ will be published on the webpages www.thp.uni-koeln.de/~gu and www.thp.uni-koeln.de/~ck.

Comparing coefficients in equation (35) yields a set of recursive differential equations for the functions $G(\ell; \underline{m}, i)$. To ease the comparison of coefficients we split a specific $\underline{m}$ with k fixed into two parts as defined by i

$$\underline{m} = (\underline{m}_l, \underline{m}_r) \tag{36}$$

with $|\underline{m}_l| = i - 1$ and $|\underline{m}_r| = k - i + 1$ such that the splitting reflects the structure of $\mathcal{O}(\underline{m}; i)$ in (34). Then the explicit recursions can be denoted by

$$\frac{\partial}{\partial \ell} G(\ell; \underline{m}; i) = \sum_{\substack{\underline{m}_l = (\underline{m}_a, \underline{m}_b) \\ \underline{m}_a \neq 0}} \mathrm{sgn}(M(\underline{m}_a)) F(\ell; \underline{m}_a) G(\ell; (\underline{m}_b, \underline{m}_r); i - |\underline{m}_a|)$$

$$- \sum_{\substack{\underline{m}_r = (\underline{m}_a, \underline{m}_b) \\ \underline{m}_b \neq 0}} \mathrm{sgn}(M(\underline{m}_b)) F(\ell; \underline{m}_b) G(\ell; (\underline{m}_l, \underline{m}_a); i). \tag{37}$$

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

$$\underline{m}_a = (m_1) \qquad \text{and} \qquad \underline{m}_b = (m_2, \ldots, m_{i-1})$$
$$\underline{m}_a = (m_1, m_2) \qquad \text{and} \qquad \underline{m}_b = (m_3, \ldots, m_{i-1})$$
$$\vdots \qquad\qquad\qquad\qquad \vdots$$
$$\underline{m}_a = (m_1, m_2, \ldots, m_{i-1}) \qquad \text{and} \qquad \underline{m}_b = (\,). \tag{38}$$

This implies that the $G(\ell; \underline{m}; i)$ appearing on the right-hand side of equation (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 $\mathcal{O}(x; \ell = 0) = \mathcal{O}$ and read

$$G(0; \underline{m}; 1) = 1 \qquad \text{for} \quad |\underline{m}| = 0 \tag{39a}$$
$$G(0; \underline{m}; i) = 0 \qquad \text{for} \quad |\underline{m}| > 0. \tag{39b}$$

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

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

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

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

$$= \mathrm{e}^{-\ell} 1 \tag{40}$$

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

$$G(\ell; (1); 2) = 1 - \mathrm{e}^{-l} \xrightarrow[\ell \to \infty]{} 1. \tag{41}$$

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

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

$$+ \text{sgn}\,[M((-2))]\,F(\ell; (-2))G(\ell; (1), 2) \tag{42a}$$
$$= -(\mathrm{e}^{-3\ell} - \mathrm{e}^{-\ell}) \cdot 1 - \mathrm{e}^{-2\ell} \cdot (1 - \mathrm{e}^{-\ell}) \tag{42b}$$
$$= \mathrm{e}^{-\ell} - \mathrm{e}^{-2\ell}. \tag{42c}$$

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

$$G(\ell; (-2, 1); 3) = -\mathrm{e}^{-\ell} + \tfrac{1}{2}\,\mathrm{e}^{-2\ell} + 1 - \tfrac{1}{2} \xrightarrow[\ell \to \infty]{} \tfrac{1}{2}. \tag{43}$$

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

$$\int_0^\ell \mathrm{d}\ell'\,\ell'^i = \frac{1}{i+1}\ell^{i+1} \tag{44a}$$

$$\int_0^\ell \mathrm{d}\ell'\,\ell'^i\,\mathrm{e}^{-2\mu\ell'} = \frac{i!}{2\mu}\left[\frac{1}{(2\mu)^i} - \mathrm{e}^{-2\mu\ell}\sum_{j=0}^{i}\frac{\ell^j}{j!(2\mu)^{i-j}}\right] \tag{44b}$$

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

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

$$G(\ell; \underline{m}; i) = G(\ell; (-m_k, \ldots, -m_1); k - i + 2) \tag{45a}$$
$$G(\ell; \underline{m}; i) = G(\ell; (-m_1, \ldots, -m_k); i)(-1)^{|\underline{m}|} \tag{45b}$$

as can be shown by induction. The first symmetry (45a) holds if $\mathcal{O}$ is Hermitian. Unfortunately, there is no equivalence to equation (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 $\tilde{C}(\underline{m}; i) := G(\infty; \underline{m}; i) \in \mathbb{Q}$ are obtained as rational numbers. So we retrieve finally

$$\mathcal{O}_{\text{eff}}(x) = \sum_{k=0}^{\infty} x^k \sum_{i=1}^{k+1} \sum_{|\underline{m}|=k} \tilde{C}(\underline{m}; i)\mathcal{O}(\underline{m}; i) \tag{46}$$

similar to equation (31). We will make the coefficients $\tilde{C}(\underline{m}; i)$ available electronically (see footnote 3). Note that $\mathcal{O}_{\text{eff}}$ is *not* a particle-conserving quantity as is obvious from the fact that the sum over $|\underline{m}|$ is not restricted to $M(\underline{m}) = 0$. 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 $\mathcal{O} = \sum_{n=-N'}^{N'} T_n'$, where T_n' increments (or decrements, if $n < 0$) the number of particles by n: $[Q, T_n'] = nT_n'$.

The difference between the bare initial observable $\mathcal{O}$ and the representation (46) must be viewed as a 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.

5. Conclusions

5.1. Summary

In this paper we have presented an approach to calculate energies and observables for quantum multi-particle systems defined on lattices. The paper has two main parts. In the first part (section 2), 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 would 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 us to compute the *n*-particle contribution for arbitrary *n*. For instance, the formulae for the three-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 (sections 3 and 4), 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 section 3 the treatment of the Hamiltonian is given. The computation of the effective Hamiltonian requires the solution of a set of recursive nonlinear 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 section 4 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 need 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, 19, 22, 24–28]. These results may serve as examples for the utility of the approach presented.

5.2. Outlook

We would 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 an 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) [29, 30]. Note that the problems linked to the existence of anomalous Green functions [30] 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 η and the observables $\mathcal{O}$, 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 two-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 $t_{j_1\ldots;i_1\ldots}$ and $\partial_\ell t_{j_1\ldots;i_1\ldots}$ in front of the terms $e^\dagger_{j_1}\ldots e_{i_1}\ldots$ yields coupled nonlinear 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 *kinds* of terms retained stay the same. Again, the formulation in second quantization allows a significant generalization. We would like to stress again that the approach presented does not require a weak-coupling limit. For illustration, however, the reader is referred to the weak-coupling examples in [5–7].

(c) *Concluding remark.* In this paper we discussed the general structure of effective operators and a perturbative unitary transformation to derive them. No concrete application is presented since such applications can be found elsewhere. The two continuative points above show along which lines the general structure can be exploited to extend the applicability beyond zero-temperature results and beyond finite range processes. Work along these lines is partly under way, but deserves definitely further attention.

Acknowledgments

Appendix. Three-particle irreducible interaction

Here we complete the formulae for the irreducible three-particle interaction which was given in equation (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

$$A_0 = E_0^A \left[\delta_{j_1 i_1} \tilde{\delta}_{j_2 j_3; i_2 i_3} + \delta_{j_1 i_2} \tilde{\delta}_{j_2 j_3; i_1 i_3} + \delta_{j_1 i_3} \tilde{\delta}_{j_2 j_3; i_1 i_2} \right] \tag{A1a}$$

$$\begin{aligned}
A_1 = {} & t_{j_1; i_1}^A \tilde{\delta}_{j_2 j_3; i_2 i_3} + t_{j_1; i_2}^A \tilde{\delta}_{j_2 j_3; i_1 i_3} + t_{j_1; i_3}^A \tilde{\delta}_{j_2 j_3; i_1 i_2} + t_{j_2; i_1}^A \tilde{\delta}_{j_1 j_3; i_2 i_3} + t_{j_2; i_2}^A \tilde{\delta}_{j_1 j_3; i_1 i_3} + t_{j_2; i_3}^A \tilde{\delta}_{j_1 j_3; i_1 i_2} \\
& + t_{j_3; i_1}^A \tilde{\delta}_{j_1 j_2; i_2 i_3} + t_{j_3; i_2}^A \tilde{\delta}_{j_1 j_2; i_1 i_3} + t_{j_3; i_3}^A \tilde{\delta}_{j_1 j_2; i_1 i_2}
\end{aligned} \tag{A1b}$$

$$\begin{aligned}
A_2 = {} & \delta_{j_1 i_1} \tilde{t}_{j_2 j_3; i_2 i_3}^A + \delta_{j_1 i_2} \tilde{t}_{j_2 j_3; i_1 i_3}^A + \delta_{j_1 i_3} \tilde{t}_{j_2 j_3; i_1 i_2}^A + \delta_{j_2 i_1} \tilde{t}_{j_1 j_3; i_2 i_3}^A + \delta_{j_2 i_2} \tilde{t}_{j_1 j_3; i_1 i_3}^A + \delta_{j_2 i_3} \tilde{t}_{j_1 j_3; i_1 i_2}^A \\
& + \delta_{j_3 i_1} \tilde{t}_{j_1 j_2; i_2 i_3}^A + \delta_{j_3 i_2} \tilde{t}_{j_1 j_2; i_1 i_3}^A + \delta_{j_3 i_3} \tilde{t}_{j_1 j_2; i_1 i_2}^A
\end{aligned} \tag{A1c}$$

where we used the shorthand

$$\tilde{\delta}_{j_1 j_2; i_1 i_2} := \delta_{j_1 i_1} \delta_{j_2 i_2} + \delta_{j_1 i_2} \delta_{j_2 i_1} \tag{A2a}$$

$$\tilde{t}_{j_1 j_2; i_1 i_2}^A := t_{j_1 j_2; i_1 i_2}^A + t_{j_1 j_2; i_2 i_1}^A + t_{j_2 j_1; i_1 i_2}^A + t_{j_2 j_1; i_2 i_1}^A. \tag{A2b}$$

While the actual formulae are lengthy the underlying principle is straightforward (see the main text). Note that in concrete realizations it is often advantageous to denote only one representative of the states which does not change on interchange of particles ($|ji\rangle = |ij\rangle$). Furthermore, certain problems allow us to exploit higher particular symmetries such as 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.

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