Perturbation Expansions for Quantum Many-Body Systems

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1   Introduction

The linked cluster method is one of the most efficient ways to generate perturbation series expansions for quantum lattice models. For the ground state energy and related properties, a linked cluster approach was first discussed in unpublished work by Nickel, followed by work of Marland [1], Irving and Hamer [2] and others, as reviewed by He et al. [3]. The approach was later rediscovered and applied to a whole new range of problems in condensed matter physics by Singh, Huse and Gelfand [4, 5].

For the energies of excited states, it is more difficult to formulate a true linked cluster expansion, although related methods have been known for some time [6]. It was only in 1996 that the key to a true linked cluster expansion for one-particle excited states was discovered by Gelfand [7]. Since then, many applications of this technique have been made, calculating single-particle energies, dispersion relations and spectral functions in models of interest in condensed matter physics. For a recent review, see Gelfand and Singh [8].

The cluster expansion method allows that the calculations can be carried out systematically and efficiently by fully automated computer programs. Furthermore, these methods work by breaking up the thermodynamic problem into a purely combinatorial problem and a number of finite-cluster problems. Thus, while they are technically harder in higher than one dimension, the difficulty is not fundamental. The combinatorial problem itself lies in an efficient treatment of the underlying clusters: Cluster data for the lattices at hand have to be generated while clusters leading to redundant calculations should be classified in terms of canonical clusters. Further a convenient handle to iterate and refer the

subclusters of a given cluster should be provided. Over the years several groups have developed computer programs to deal with these problems [8, 9, 10]. An approach using object-oriented programming tools and highly efficient algorithms from graph theory has been presented in [11].

Conceptually, our new approach is a generalization of Gelfand's linked cluster expansion for single-particle excited states to two-particle states [12]. From a technical point of view, the development of an orthogonality transformation now enables a linked cluster theorem for multi-particle states even when their quantum numbers are identical with the ground state [13]. We show how to calculate energies and dispersion relations for two-particle excitations, and coherence lengths for the bound states.

2 Formalism

We consider a Hamiltonian

$$H = H_0 + \lambda H_1 \ , \tag{1}$$

where the unperturbed Hamiltonian H_0 is exactly solvable, and λ is the perturbation parameter. In the lattice models of interest, H_0 will typically consist of single-site operators, while interaction terms between different sites will be included in the perturbation operator H_1. Our aim is to calculate perturbation series in λ for the eigenvalues of H and other quantities of interest. This scenario of an expansion around a local Hamiltonian is in contrast to the case of free particles with non-local, infinitely extended states. Here, one might apply Wick's theorem to construct a perturbation theory.

In the following we will review the procedure for ground state properties and single-particle excitations and present an extended formalism to study two-particle excitations. The calculation generally proceeds in three stages, block diagonalization, linked cluster expansion and calculation of eigenvalues.

2.1 Block Diagonalization

On any finite lattice or cluster of sites, the first step is to block diagonalize the Hamiltonian to form an effective Hamiltonian, where the ground state is in a block by itself, the one-particle states form another block, the two-particle states another block, and so on. Here a particle may refer to a spin-flip, a lattice

fermion, or other excitation, depending on the model at hand. We assume that all the unperturbed states in each block are degenerate under H_0.

In the following we will present a procedure to generate these effective Hamiltonians in the respective particle sectors order by order. We present a recursive formulation of Rayleigh-Schrödinger perturbation theory which can be easily implemented.

To calculate ground state properties is almost trivial as one can apply non-degenerate perturbation theory. For single particle excitations a similarity transformation can be applied to block diagonalize the effective Hamiltonian, since the excited state and the ground state usually have non-identical quantum numbers. This is in contrast to the case of two-particle excitations which may be described by the same quantum numbers as the ground state. This situation requires a more elaborated block diagonalization in terms of an orthogonal transformation.

2.1.1   Ground state energy

We start with a cluster Hamiltonian H of the form

$$H = H_0 + \lambda H_1 \ ,$$

where all Hamiltonians are restricted to act on the Hilbert space associated with the cluster at hand. We assume that there exists a ground state of the unperturbed Hamiltonian H_0 which is unique allowing us to apply a non degenerate perturbation theory.

The assumption of a unique ground state does not imply that this ground state has to be non degenerate. It rather denotes that the application of the perturbative Hamiltonian H_1 does not transfer a chosen ground state to a degenerate one.

Expanding the ground state energy E_0 and the unnormalized ground state wave vector $|\psi\rangle$ in λ gives

$$
\begin{aligned}
E &= \sum_{n=0}^{\infty} \lambda^n e_n \\
|\psi\rangle &= \sum_{n=0}^{\infty} \lambda^n |\psi_n\rangle \ .
\end{aligned}
\tag{2}
$$

Inserting these expansions into the Schrödinger equation gives

$$H|\psi\rangle = E|\psi\rangle$$

$$\sum_{n=0} H_0 \lambda^n |\psi_n\rangle + \sum_{n=1} H_1 \lambda^n |\psi_{n-1}\rangle = \sum_{n=0} \lambda^n \sum_{m=0}^{n} e_m |\psi_{n-m}\rangle . \qquad (3)$$

Collecting all terms of order λ^n we find

$$H_0 |\psi_n\rangle + H_1 |\psi_{n-1}\rangle = \sum_{m=0}^{n} e_m |\psi_{n-m}\rangle . \qquad (4)$$

We now choose a particularly convenient normalization condition of the form

$$\langle \psi_0 | \psi_n \rangle = \delta_{0n} , \qquad (5)$$

which will give the recursion relations

$$e_n = \langle \psi_0 | H_1 | \psi_{n-1} \rangle \qquad (6)$$

$$\langle k | \psi_n \rangle = \frac{1}{E_0 - E_k} \left(\langle k | H_1 | \psi_{n-1} \rangle - \sum_{m=1}^{n-1} e_m \langle k | \psi_{n-m} \rangle \right) , \qquad (7)$$

where $|k\rangle$ denotes any basis state but the ground state and $E_k = \langle k | H_0 | k \rangle$ is the corresponding energy.

The occurrence of the ratios $\frac{1}{E_0 - E_k}$ strongly determines the convergence of the generated series. If the energy gap to the elementary excitation vanishes the ratios will diverge and the calculated series is not expected to show a good convergence and vice versa.

2.1.2 Single-particle excitation: Similarity transformation

Gelfand [7] showed that by means of a linked cluster expansion one can efficiently generate high-order expansions which directly give the Fourier series coefficients of the dispersion of the low-lying excitations. The numerical calculations involved are straightforward extensions of those previously described to generate ground state energy expansions.

Again, we consider a Hamiltonian

$$H = H_0 + \lambda H_1 ,$$

in which the unperturbed Hamiltonian H_0 is trivially diagonalizable and of fixed degeneracy on any finite cluster.

The new approach that is based on the construction of an effective Hamiltonian within a degenerate manifold of excited states for each finite cluster with respect to some unperturbed Hamiltonian H_0. Let us assume that there are L degenerate states out of M states total and that the eigenstates of H_0 are ordered in a way that the first L states are those of the degenerate manifold. We can choose a similarity transformation S so that in H^{eff} there are vanishing matrix elements between the states of the degenerate manifold, that is, S equals the identity matrix within the upper left $L \times L$ block. By doing so, H^{eff} breaks up onto an $L \times L$ block in the upper left, $H^{\text{eff}}(1)$, describing the interactions between the degenerated states of the manifold, and an $(M - L) \times (M - L)$ block, describing all the other physics of the cluster

$$
S^{-1}HS = \begin{pmatrix} \boxed{H^{\text{eff}}(1)} & 0 \\ 0 & \boxed{\cdots} \end{pmatrix} . \tag{8}
$$

We can think of the similarity transformation S as a set of column vectors $\left(\psi^{(l)}\right)$. Rewriting equation (8) as

$$
HS = SH^{\text{eff}} \tag{9}
$$

gives an equation where the vectors $\psi^{(l)}$ with $1 \leq l \leq L$ are not coupled to those with $L + 1 \leq l \leq M$. In order to calculate H^{eff} we can thus neglect the lower right $(M - L) \times (M - L)$ block of H^{eff}. To this end, we now expand $\psi^{(l)}$ and H^{eff} in terms of λ

$$
\begin{aligned}
\psi^{(l)} &= \sum_n \lambda^n \psi_n^{(l)} \\
H^{\text{eff}}(l', l) &= \sum_n \lambda^n H_n^{\text{eff}}(l', l) .
\end{aligned} \tag{10}
$$

Inserting these expansions in equation (9) and collecting all terms of order λ^n gives

$$
H_0 \psi_n^{(l)} + H_1 \psi_{n-1}^{(l)} = \sum_{m=0}^{n} \sum_{l'=1}^{L} \psi_m^{(l')} H_{n-m}^{\text{eff}}(l', l) . \tag{11}
$$

5

We now choose a normalization convention of the form

$$\langle l|\psi_n^{(l')}\rangle = \delta_{n,0}\delta_{l,l'} \ , \tag{12}$$

which gives us the desired recursive relations

$$
\begin{aligned}
H_n^{\text{eff}}(m,l) &= \langle m|H_1|\psi_{n-1}^{(l)}\rangle \tag{13}\\
\langle k|\psi_n^{(l)}\rangle &= \frac{1}{E_0 - E_k}\left(\langle k|H_1|\psi_{n-1}^{(l)}\rangle - \sum_{m=1}^{n-1}\sum_{l'=1}^{L} H_{n-m}^{\text{eff}}(l',l)\langle k|\psi_m^{(l')}\rangle\right) \tag{14}
\end{aligned}
$$

Here $|k\rangle$ is a state out of the degenerate manifold and E_k is the corresponding unperturbed energy $E_k = \langle k|H_0|k\rangle$. These recursion relations for the excited states are very similar to those obtained in the development of the ground state energy in equation (7). It is reasonable that the computer code written for the ground state expansion can be easily extended to study the first excited state as well.

2.1.3 Two-particle excitation: Orthogonal transformation

We developed a generalization of the single-particle approach to block diagonalize the Hamiltonian in order to calculate an effective Hamiltonian for two-particle excitations. In this case, we also intend to transform the Hamiltonian so that we obtain a block structure with the ground state sitting in a block $H^{\text{eff}}(0)$, the one-particle states form another block $H^{\text{eff}}(1)$, the two-particle states another block $H^{\text{eff}}(2)$, and so on:

$$
O^T H O = H^{\text{eff}} =
\begin{pmatrix}
\boxed{H^{\text{eff}}(0)} & 0 & 0 & 0 \\
0 & \boxed{H^{\text{eff}}(1)} & 0 & 0 \\
0 & 0 & \boxed{H^{\text{eff}}(2)} & 0 \\
0 & 0 & 0 & \boxed{\cdots} \\
\underbrace{\hspace{1.5cm}}_{\substack{\text{ground state}\\\text{block}}} & \underbrace{\hspace{1.5cm}}_{\substack{1-\text{particle}\\\text{block}}} & \underbrace{\hspace{1.5cm}}_{\substack{2-\text{particle}\\\text{block}}} &
\end{pmatrix}
\ . \tag{15}
$$

While Gelfand used a similarity transformation we need to apply a *unitary* transformation in order to preserve all the proper symmetries of the Hamiltonian in the two-particle case. This is due to the circumstance that a two-particle excitation may be classified by the same quantum numbers as the ground state. For example, one may consider a spin system with a singlet ground state where two triplet excitations can form a singlet state again. Here we will only account for the case when the Hamiltonian is real and symmetric, and can be block diagonalized by an *orthogonal* transformation O.

The orthogonality of O can be ensured by writing

$$O = e^S \ , \tag{16}$$

where S is real and antisymmetric

$$S^T = -S \ . \tag{17}$$

This transformation is again constructed order by order in perturbation theory. The matrix elements of H^{eff} between different blocks are zero, up to the given order in perturbation theory. Each matrix is expanded in powers of λ:

$$O = \sum_{n=0}^{\infty} \lambda^n O_n \ , \tag{18}$$

$$S = \sum_{n=0}^{\infty} \lambda^n S_n \ , \tag{19}$$

$$H^{\text{eff}} = \sum_{n=0}^{\infty} \lambda^n H_n^{\text{eff}} \ , \tag{20}$$

where at zeroth order we set

$$S_0 = 0, \quad O_0 = I, \quad H_0^{\text{eff}} = H_0 \ . \tag{21}$$

Here I is the unit matrix, H_0 is a diagonal matrix, with diagonal matrix elements E_0^i.

At higher orders $n \neq 0$, we have

$$O_n = S_n + \frac{1}{2} \sum_{m,l=1}^{n} S_m S_l \delta_{m+l,n} + \frac{1}{3!} \sum_{m,l,k=1}^{n} S_m S_l S_k \delta_{m+l+k,n} + ... \tag{22}$$

$$H_n^{\text{eff}} = \begin{pmatrix} \boxed{} & 0 & 0 \\ 0 & \boxed{} & 0 \\ 0 & 0 & \boxed{} \end{pmatrix} \qquad\qquad S_n = \begin{pmatrix} 0 & \boxed{} & \boxed{} \\ \boxed{} & 0 & \boxed{} \\ \boxed{} & \boxed{} & 0 \end{pmatrix}$$

Figure 1: Block structure of the matrices H_n^{eff} and S_n. Setting the upper right blocks of H_n^{eff} to zero determines the corresponding (shaded) blocks of S_n. The diagonal blocks of S_n are set to zero.

and

$$\sum_{m,l=0}^{n} O_m H_l^{\text{eff}} \delta_{m+l,n} = H_0 O_n + H_1 O_{n-1} \,, \tag{23}$$

where it is convenient to define

$$R_n = O_n - S_n \,. \tag{24}$$

If we demand that at any given order n the off-diagonal blocks of H_n^{eff} vanish in (say) the upper right triangle, then the entries in the corresponding blocks of S_n are determined by equation (23). The block structure of these matrices is illustrated in Fig. 1. The transposed blocks in the lower left triangle are then determined by the antisymmetry condition (17) and only the diagonal blocks of S remain to be determined. The simplest choice is to set the diagonal blocks to zero. Thus, S_n is completely determined by

$$S_n^{(ij)} = -R_n^{(ij)} + \frac{1}{E_0^{(j)} - E_0^{(i)}} \left(H_1 O_{n-1} - \sum_{m,l=1}^{n-1} O_m H_l^{\text{eff}} \delta_{m+l,n} \right)^{(ij)} \tag{25}$$

and

$$O_n^{(ij)} = \frac{1}{E_0^{(j)} - E_0^{(i)}} \left(H_1 O_{n-1} - \sum_{m,l=1}^{n-1} O_m H_l^{\text{eff}} \delta_{m+l,n} \right)^{(ij)} \tag{26}$$

for elements (ij) in the off-diagonal (shaded) blocks. The diagonal blocks of H_n^{eff}) are then obtained as

$$(H_n^{\text{eff}})^{(ij)} = \{ H_1 O_{n-1} - \sum_{m,l=1}^{n-1} O_m H_l^{\text{eff}} \delta_{m+l,n} \}^{(ij)} \,. \tag{27}$$

8

The right-hand sides of equations (25),(26), and (27) can be computed recursively from the results at order $(n-1)$.

The key differences from the similarity transformation are as follows. In the similarity transformation, the diagonal blocks of S_n are undetermined, and so are chosen to be zero, while the off-diagonal blocks of S_n are antisymmetric and can be determined by demanding the off-diagonal blocks of H_n^{eff} to be zero. In the orthogonal transformation, on the other hand, the diagonal blocks of O_n cannot be chosen to be zero. Instead the diagonal blocks of S_n are chosen to be zero, while the diagonal blocks of O_n are required to be nonzero by orthogonality, and are determined by Eq. (22).

At the end of this process, the effective Hamiltonian has been block diagonalized, up to a given order in perturbation theory. The orthogonal transformation will turn the unperturbed two-particle states into dressed states containing admixtures of different particle numbers. In particular, there will be no annihilation process for these dressed states. The states will still be labeled by the positions of the original unperturbed particles, though they will contain admixtures of other particle states at n earby locations.

At any finite order in perturbation theory, we may assume that the effective Hamiltonian will remain local (that is, interactions between states do not extend beyond a finite range) and will have the same bulk symmetries as the original Hamiltonian, such as translation symmetry. These properties are sufficient to admit a linked cluster approach to the calculation of eigenvalues.

We note that the solution of the equations above is not nearly as efficient as the similarity transformation of Gelfand. In particular, the solution of the equation (22) is expensive in CPU time and memory.

2.2 Linked Cluster Expansions

In order to obtain a strong coupling cluster expansion we consider problems where H_0 and H_1 can be expressed as a sum of various local terms

$$H = \sum_k h_k \; . \tag{28}$$

The index k runs over all pairs of lattice sites that are connected by some interaction which can be expressed by local operators. For example, in a spin model a nearest neighbor interaction can be modeled by an interaction term $\sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j$, or by a kinetic term $\sum_{\langle ij \rangle} c_i^\dagger c_j$ in a fermionic model. Here, the generic index k is replaced by the index $\langle ij \rangle$ that runs over all nearest neighbor pairs.

Let P be a generic extensive property to be studied by a cluster expansion. For the development of a cluster expansion, we associate each term in H_1 with an individual coefficient λ_k. We can then rewrite P as a formal multivariable expansion in powers of the λ_k

$$P(\{\lambda_k\}) = \sum_{\{n_k\}} p\{n_k\} \prod_k {\lambda_k}^{n_k} \; , \tag{29}$$

where each of the n_k runs over all non-negative integers.

A cluster C is a non-empty set of indices k. Thus, a cluster is a set of connected sites, but not necessarily connected itself. By reorganizing the terms in equation (29), one can formulate a cluster expansion

$$P(\{\lambda_k\}) = \sum_C W_{[P]}(C) \; . \tag{30}$$

The cluster weight $W_{[P]}(C)$ contains all terms in the former multivariable expansion for P in equation (29) which have at least one power of λ_k for all the indices k in the actual cluster and no powers of any other λ_k. The cluster weight $W_{[P]}(C)$ can be calculated by inverting equation (30)

$$W_{[P]}(C) = P(C) - \sum_{C' \subset C} W_{[P]}(C') \; . \tag{31}$$

Thus, the cluster weight is given by calculating the property $P(C)$ on the cluster C and subtracting all the weights of the subclusters C' of C.

The crucial feature of the cluster weights is that if a cluster C contains n edges, that is that there are n indices of terms in H_1, it will contribute first in
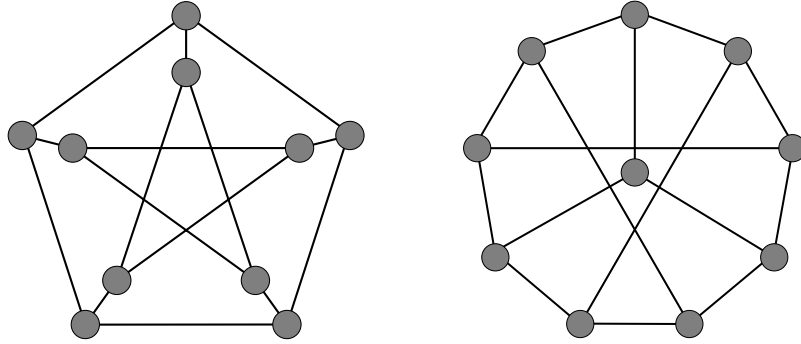
Figure 2: Two equivalent graphs.

order λ^n. The explicit subtraction of subclusters sets all coefficients of λ^0, λ^1, ..., λ^{n-1} to zero. Thus, to obtain an expansion of P/N which is correct to order n one has to sum up the cluster weights only from clusters with up to n edges. Here N is the system size.

2.2.1 Canonical clusters

By explicitely defining a multivariable expansion we have introduced the concept of a cluster expansion. Now we can simplify the above expansions by setting all λ_k equal to λ. Topologically equivalent clusters will then give identical contributions to the expansion.

Two clusters G and H are called (topologically) equivalent if there is a mapping M of the vertices of G to the vertices of H such that $M(G)$ and H are identical. Clusters related by basic symmetries such as translations and various reflections are obviously equivalent by this definition.

In the following we will identify sets of equivalent clusters by a single canonical representative $\tilde{C}$. The number of clusters from this set covering an arbitrary (but fixed) site on the infinite lattice is called the lattice constant[1] of the cluster, $L(\tilde{C})$. Thus, the lattice constant equals the number of embeddings of the cluster $\tilde{C}$ on the underlying lattice.

In terms of canonical representatives the cluster expansion for the property

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[1]This lattice constant reflecting geometric properties of a cluster embedded on a lattice is not to be confused with the lattice constant describing the lattice spacing.

P on the infinite lattice is expressed as

$$P(\lambda)/N = \sum_{\tilde{C}} L(\tilde{C}) \cdot W_{[P]}(\tilde{C}) \,, \tag{32}$$

where N is the system size.

2.2.2 Linked cluster theorem

For a number of ground state properties it turns out that disconnected clusters have vanishing cluster weights and only a finite number of connected clusters has to be considered in the actual expansion.

In general, properties that are additive for disjoint unions of non-empty clusters have a connected or linked cluster expansion. The linked cluster theorem is given by

$$P_C = P_A + P_B \quad \Rightarrow \quad W_{[P]}(C) = 0 \,, \tag{33}$$

which is easily proved by the following argument

$$
\begin{aligned}
W_{[P]}(C) &= P_C - \sum_{C' \subset C} W_{[P]}(C') \\
&= P_A - \sum_{C' \subseteq A} W_{[P]}(C') + P_B - \sum_{C' \subseteq B} W_{[P]}(C') \\
&= 0 \,.
\end{aligned}
$$

A cluster is called disconnected if the cluster Hamiltonian H_C can be expressed as a sum of disjoint subcluster Hamiltonians acting on direct product spaces

$$H_C = H_A \otimes I_B + I_A \otimes H_B \,, \tag{34}$$

where I_A and I_B are identity operators on the subclusters A and B. The ground state wavefunction for such a disconnected cluster C can be written as

$$|\psi_C\rangle = |\psi_A\rangle \otimes |\psi_B\rangle \,. \tag{35}$$

This directly implies that the ground state energy obeys the linked cluster theorem and that there is a linked cluster expansion for the ground state energy.

Let us now briefly summarize the linked cluster approach in various particle sectors.
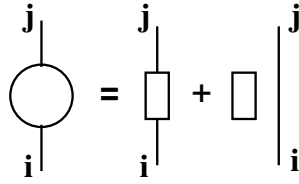
Figure 3: Decomposition of a one-particle matrix element into irreducible components as given by equation (40). The round box denotes the full matrix element, the square boxes the irreducible matrix elements, and the single line denotes a delta function.

2.2.3 Ground state energy

The ground state energy E_0 is a simple extensive quantity which obeys the linked cluster theorem (33), that is:

$$E_0^C = E_0^A + E_0^B \, , \tag{36}$$

where E_0^C is the ground state energy on a cluster C composed of two disconnected subclusters A and B. Thus, one can perform a linked cluster expansion as outlined above [2, 5]. An efficient recursive algorithm to generate a perturbation series for the ground state energy involves the following steps:

i) Generate a list of canonical clusters $\{\tilde{C}\}$, along with their lattice constants $L(\tilde{C})$, appropriate to the problem at hand [11];

ii) For each cluster $\tilde{C}$, the diagonal entry in the 0-particle sector of H^{eff} gives a perturbation series for the energy $E_0^{\tilde{C}}$;

iii) Calculate the cluster weight $W_{[E_0]}(\tilde{C})$ by subtracting all subcluster contributions to $E_0(\tilde{C})$ according to equation (31);

iv) Summarize all cluster weights as in equation (32) to obtain the desired perturbation series for E_0.

2.2.4 One-particle excited states

It turns out that the effective Hamiltonian constructed by a similarity transformation (see previous section) is not an additive property obeying the linked cluster

theorem (33). For a cluster C that is the disjoint union of the subcluster A and B

$$H_C^{\text{eff}} = \left[H^{\text{eff}} + e_B I\right]_A \oplus \left[H^{\text{eff}} + e_A I\right]_B \neq H_A^{\text{eff}} \oplus H_B^{\text{eff}} , \qquad (37)$$

where e_A denotes the ground state energy of cluster A and I is the identity operator. Thus, H^{eff} itself does not have a cluster expansion.

Gelfand [7] demonstrated how to generalize the method to one-particle excited states. Let

$$E_1(\mathbf{i},\mathbf{j}) = \langle \mathbf{j}|H^{\text{eff}}(1)|\mathbf{i}\rangle \qquad (38)$$

be the matrix element of H^{eff} between initial one-particle state $|\mathbf{i}\rangle$ and final one-particle state $|\mathbf{j}\rangle$, labeled according to their positions on the lattice. The excited state energy is not extensive and does not obey the cluster addition property, but there is a related quantity which does. If cluster C is made up of disconnected subclusters A and B, and states $|\mathbf{i}\rangle$ and $|\mathbf{j}\rangle$ reside on cluster A, then

$$E_1^C(\mathbf{i},\mathbf{j}) = E_1^A(\mathbf{i},\mathbf{j}) + E_0^B . \qquad (39)$$

However, if we define the irreducible one-particle matrix element (Fig. 3)

$$\Delta_1(\mathbf{i},\mathbf{j}) = E_1(\mathbf{i},\mathbf{j}) - E_0 \delta_{\mathbf{i},\mathbf{j}} , \qquad (40)$$

it is given by

$$\Delta_1^C(\mathbf{i},\mathbf{j}) = \Delta_1^A(\mathbf{i},\mathbf{j}) , \qquad (41)$$

whereas if $|\mathbf{i}\rangle$ and $|\mathbf{j}\rangle$ reside on cluster B, we obtain

$$\Delta_1^C(\mathbf{i},\mathbf{j}) = \Delta_1^B(\mathbf{i},\mathbf{j}) , \qquad (42)$$

or in general

$$\Delta_1^C(\mathbf{i},\mathbf{j}) = \Delta_1^A(\mathbf{i},\mathbf{j}) + \Delta_1^B(\mathbf{i},\mathbf{j}) , \qquad (43)$$

where $\Delta_1(\mathbf{i},\mathbf{j})$ *vanishes* for any cluster not containing $\mathbf{i}$ and $\mathbf{j}$. Note that a one-particle state cannot vanish on one subcluster and reappear on the other, after the initial block diagonalization.

From the cluster addition property (43) it follows that the elements $\Delta_1(\mathbf{i},\mathbf{j})$ can be expanded in terms of contributions from *connected* clusters alone. They can be calculated efficiently by an analogous algorithm to the one outlined for the ground state energy.
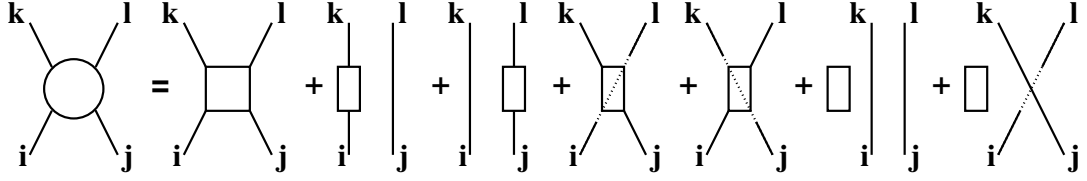
Figure 4: Decomposition of two identical particle matrix element into irreducible components as given by equation (45). Notation as in Fig. 3

2.2.5 Two-particle states

The generalization to two-particle states is now a straight forward extension. Let

$$E_2(\mathbf{i}, \mathbf{j}; \mathbf{k}, \mathbf{l}) = \langle \mathbf{k}, \mathbf{l} | H^{\text{eff}}(2) | \mathbf{i}, \mathbf{j} \rangle \tag{44}$$

be the matrix element between initial two-particle state $|\mathbf{i}, \mathbf{j}\rangle$ and final state $|\mathbf{k}, \mathbf{l}\rangle$. To obtain a quantity obeying the cluster addition property, we must subtract the ground state energy and one-particle contributions, to form the irreducible two-particle matrix element [Fig. 4]:

$$
\begin{aligned}
\Delta_2(\mathbf{i}, \mathbf{j}; \mathbf{k}, \mathbf{l}) &= E_2(\mathbf{i}, \mathbf{j}; \mathbf{k}, \mathbf{l}) - E_0(\delta_{\mathbf{i},\mathbf{k}}\delta_{\mathbf{j},\mathbf{l}} + \delta_{\mathbf{i},\mathbf{l}}\delta_{\mathbf{j},\mathbf{k}}) - \Delta_1(\mathbf{i}, \mathbf{k})\delta_{\mathbf{j},\mathbf{l}} - \Delta_1(\mathbf{i}, \mathbf{l})\delta_{\mathbf{j},\mathbf{k}} \\
&\quad - \Delta_1(\mathbf{j}, \mathbf{k})\delta_{\mathbf{i},\mathbf{l}} - \Delta_1(\mathbf{j}, \mathbf{l})\delta_{\mathbf{i},\mathbf{k}} \ .
\end{aligned}
\tag{45}
$$

This quantity is easily found to be *zero* for any cluster unless **i, j, k** and **l** are all included in that cluster and it meets the cluster addition property. Once again, the block diagonalization ensures that two particles cannot vanish from one cluster and reappear on another disconnected one. Thus, the matrix elements of Δ_2 can be expanded in terms of connected clusters alone, which are rooted or connected to all four positions **i, j, k, l**.

2.3 Calculation of eigenvalues

While the ground state energy was directly obtained as a series in the previous subsection, the determination of energies of the excited states still needs some further calculations. To this end, the Schrödinger equation has to be solved for the excited states, that is the effective Hamiltonians in the respective degenerate manifolds need to be diagonalized. While this can be done by a simple Fourier transformation in the one-particle sector a more sophisticated procedure needs

to implemented in the two-particle case. We will discuss the solution of the two-particle Schrödinger equation by using an integral equation in momentum space or alternatively by a finite lattice approach in coordinate space.

2.3.1 One-particle states

The one-particle effective Hamiltonian can be diagonalized by a Fourier transformation. We thereby obtain a series expansion of the dispersion relation in momentum space. Assuming a homogeneous system

$$\Delta_1(\mathbf{i}, \mathbf{j}) \equiv \Delta_1(\boldsymbol{\delta}) \, , \tag{46}$$

where $\boldsymbol{\delta}$ is the difference between positions $\mathbf{i}$ and $\mathbf{j}$, translation invariance implies that the momentum $\mathbf{K}$ is a good quantum number. The corresponding eigenstate is obtained as:

$$|\mathbf{K}\rangle = \frac{1}{\sqrt{N}} \sum_{\mathbf{j}} \exp(i\mathbf{K} \cdot \mathbf{j}) |\mathbf{j}\rangle \, , \tag{47}$$

where N is the number of sites in the lattice. A Fourier transformation of the effective one-particle Hamiltonian

$$H^{\text{eff}}(|\mathbf{K}\rangle) = \sum_{\delta} e^{i\mathbf{K} \cdot \delta} H^{\text{eff}}(\mathbf{r}) \, , \tag{48}$$

will then yield the dispersion of the one-particle excitation, $\epsilon_1(\mathbf{K})$ as

$$\epsilon_1(\mathbf{K}) = \sum_{\boldsymbol{\delta}} \Delta_1(\boldsymbol{\delta}) \cos(\mathbf{K} \cdot \boldsymbol{\delta}) \, . \tag{49}$$

Here we have assumed that $\Delta_1(\boldsymbol{\delta})$ is inversion symmetric, so that

$$\Delta_1(-\boldsymbol{\delta}) = \Delta_1(\boldsymbol{\delta}) \, . \tag{50}$$

2.3.2 Two-particle states: Integral equation in momentum space

The calculation of the eigenvalues in the two-particle sector requires a more elaborated implementation. First, we describe a procedure to obtain an integral equation in momentum space. This approach is similar to one used by Mattis [14].

Consider an unsymmetrized state of non-identical particles, types a and b. Then there are $N(N-1)$ states on an N-site lattice, labeled by positions $|\mathbf{i}, \mathbf{j}\rangle$,

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where **i, j** refer to the positions of particles a and b, respectively. We have assumed here that two particles may not reside at the same position (the results are easily amended if this is not the case). Then the irreducible two-particle matrix element is

$$\Delta_2^{ab}(\mathbf{i}, \mathbf{j}; \mathbf{k}, \mathbf{l}) = E_2^{ab}(\mathbf{i}, \mathbf{j}; \mathbf{k}, \mathbf{l}) - E_0 \delta_{\mathbf{i}, \mathbf{k}} \delta_{\mathbf{j}, \mathbf{l}} - \Delta_1^a(\mathbf{i}, \mathbf{k}) \delta_{\mathbf{j}, \mathbf{l}} - \Delta_1^b(\mathbf{j}, \mathbf{l}) \delta_{\mathbf{i}, \mathbf{k}} . \quad (51)$$

Let the two-particle eigenstate be

$$|\psi\rangle = \sum_{\mathbf{i}, \mathbf{j}} f_{\mathbf{ij}} |\mathbf{i}, \mathbf{j}\rangle, \quad (i \neq j) , \quad (52)$$

which can be substituted in the Schrödinger equation

$$H^{\text{eff}} |\psi\rangle = E |\psi\rangle . \quad (53)$$

By taking the overlap with $\langle \mathbf{i}, \mathbf{j} |$ one obtains

$$(E - E_0) f_{\mathbf{ij}} - \sum_{\mathbf{k} \neq \mathbf{j}} \Delta_1^a(\mathbf{k}, \mathbf{i}) f_{\mathbf{kj}} - \sum_{\mathbf{k} \neq \mathbf{i}} \Delta_1^b(\mathbf{k}, \mathbf{j}) f_{\mathbf{ik}} = \sum_{\mathbf{k}, \mathbf{l}} \Delta_2^{ab}(\mathbf{k}, \mathbf{l}; \mathbf{i}, \mathbf{j}) f_{\mathbf{kl}} , \quad (\mathbf{i} \neq \mathbf{j}) . \quad (54)$$

The completion of the sums on the left-hand side leads to

$$(E - E_0) f_{\mathbf{ij}} - \sum_{\mathbf{k}} [\Delta_1^a(\mathbf{k}, \mathbf{i}) f_{\mathbf{kj}} + \Delta_1^b(\mathbf{k}, \mathbf{j}) f_{\mathbf{ik}}]$$
$$= \sum_{\mathbf{k}, \mathbf{l}} \Delta_2^{a,b}(\mathbf{k}, \mathbf{l}; \mathbf{i}, \mathbf{j}) f_{\mathbf{kl}} - \Delta_1^a(\mathbf{j}, \mathbf{i}) f_{\mathbf{jj}} - \Delta_1^b(\mathbf{i}, \mathbf{j}) f_{\mathbf{ii}} , \quad (55)$$

The fictitious amplitudes $f_{\mathbf{ii}}$ are introduced to simplify the calculations, and are taken to be *defined* by these equations [14].

Now we define a center-of-mass position coordinate

$$\mathbf{R} = \frac{1}{4}(\mathbf{i} + \mathbf{j} + \mathbf{k} + \mathbf{l}) , \quad (56)$$

and relative coordinates

$$\begin{aligned}
\mathbf{r} &= \frac{1}{2}(\mathbf{i} + \mathbf{j} - \mathbf{k} - \mathbf{l}) , \\
\boldsymbol{\delta}_1 &= \mathbf{i} - \mathbf{j} , \\
\boldsymbol{\delta}_2 &= \mathbf{k} - \mathbf{l} .
\end{aligned} \quad (57)$$

Furthermore, translation invariance implies that

$$\Delta_2(\mathbf{i},\mathbf{j};\mathbf{k},\mathbf{l}) \equiv \Delta_2(\mathbf{r},\boldsymbol{\delta_1},\boldsymbol{\delta_2}) \;. \tag{58}$$

Next, perform a Fourier transformation,

$$f(\mathbf{K},\mathbf{q}) = \frac{1}{N}\sum_{\mathbf{i},\mathbf{j}} e^{i(\mathbf{k_1}\cdot\mathbf{i}+\mathbf{k_2}\cdot\mathbf{j})} f_{\mathbf{ij}} \;, \tag{59}$$

where $\mathbf{K},\mathbf{q}$ are the center-of-mass and relative momenta

$$
\begin{aligned}
\mathbf{K} &= (\mathbf{k}_1 + \mathbf{k}_2) \;, \\
\mathbf{q} &= \frac{1}{2}(\mathbf{k}_1 - \mathbf{k}_2) \;.
\end{aligned} \tag{60}
$$

Inserting the relative coordinates and momenta into equation (55) we obtain the generic form of the integral equation

$$
\left(E - E_0 - \sum_{\boldsymbol{\delta}} \Delta_1^a(\boldsymbol{\delta})\cos(\mathbf{K}\cdot\boldsymbol{\delta}/2 + \mathbf{q}\cdot\boldsymbol{\delta}) + \Delta_1^b(\boldsymbol{\delta})\cos(\mathbf{K}\cdot\boldsymbol{\delta}/2 - \mathbf{q}\cdot\boldsymbol{\delta}) \right) f(\mathbf{K},\mathbf{q})
$$
$$
= \frac{1}{N}\sum_{\mathbf{q}'} f(\mathbf{K},\mathbf{q}') \left(\sum_{\mathbf{r},\boldsymbol{\delta_1},\boldsymbol{\delta_2}} \Delta_2^{ab}(\mathbf{r},\boldsymbol{\delta_1},\boldsymbol{\delta_2})\cos(\mathbf{K}\cdot\mathbf{r} + \mathbf{q}\cdot\boldsymbol{\delta_1} - \mathbf{q}'\cdot\boldsymbol{\delta_2}) \right.
$$
$$
\left. - \sum_{\boldsymbol{\delta}} \Delta_1^a(\boldsymbol{\delta})\cos(\mathbf{K}\cdot\boldsymbol{\delta}/2 + \mathbf{q}\cdot\boldsymbol{\delta}) + \Delta_1^b(\boldsymbol{\delta})\cos(\mathbf{K}\cdot\boldsymbol{\delta}/2 - \mathbf{q}\cdot\boldsymbol{\delta}) \right) \;,
$$

$$\tag{61}$$

where we have again assumed inversion symmetry

$$
\begin{aligned}
\Delta_1^{a,b}(\boldsymbol{\delta}) &= \Delta_1^{a,b}(-\boldsymbol{\delta}) \;, \\
\Delta_2^{ab}(\mathbf{r},\boldsymbol{\delta_1},\boldsymbol{\delta_2}) &= \Delta_2^{ab}(-\mathbf{r},-\boldsymbol{\delta_1},-\boldsymbol{\delta_2}) \;.
\end{aligned} \tag{62}
$$

Finally, we can simplify the integral equation (61) by considering definite *exchange symmetries* of the two-particle states. We will take into account symmetric and antisymmetric states as well as the case of identical particles.

Symmetric states

For symmetric states the amplitudes of the two-particle states obey

$$f_{ij} = +f_{ji} \qquad (63)$$

and therefore

$$f(\mathbf{K}, \mathbf{q}) = +f(\mathbf{K}, -\mathbf{q}) \ . \qquad (64)$$

Averaging over $f(\mathbf{K}, \pm\mathbf{q})$ (i.e. taking $\frac{1}{2}[f(\mathbf{K}, \mathbf{q}) + f(\mathbf{K}, -\mathbf{q})]$) the integral equation (61) is simplified as

$$\left(E - E_0 - \sum_{\boldsymbol{\delta}} [\Delta_1^a(\boldsymbol{\delta}) + \Delta_1^b(\boldsymbol{\delta})] \cos(\mathbf{K} \cdot \boldsymbol{\delta}/\mathbf{2}) \cos(\mathbf{q} \cdot \boldsymbol{\delta}) \right) f(\mathbf{K}, \mathbf{q}) \ =$$

$$\frac{1}{N} \sum_{\mathbf{q}'} f(\mathbf{K}, \mathbf{q}') \left(\sum_{\mathbf{r}, \boldsymbol{\delta_1}, \boldsymbol{\delta_2}} \Delta_2^{ab}(\mathbf{r}, \boldsymbol{\delta_1}, \boldsymbol{\delta_2}) \cos(\mathbf{K} \cdot \mathbf{r}) \cos(\mathbf{q} \cdot \boldsymbol{\delta_1}) \cos(\mathbf{q}' \cdot \boldsymbol{\delta_2}) \right.$$

$$\left. - \sum_{\boldsymbol{\delta}} [\Delta_1^a(\boldsymbol{\delta}) + \Delta_1^b(\boldsymbol{\delta})] \cos(\mathbf{K} \cdot \boldsymbol{\delta}/2) \cos(\mathbf{q} \cdot \boldsymbol{\delta}) \right) \ . \quad (65)$$

Antisymmetric states

For antisymmetric states the amplitudes of the two-particle states we use

$$f_{ij} = -f_{ji} \qquad (66)$$

which implies

$$f(\mathbf{K}, \mathbf{q}) = -f(\mathbf{K}, -\mathbf{q}) \ . \qquad (67)$$

Averaging over $f(\mathbf{K}, \pm\mathbf{q})$ (i.e. taking $\frac{1}{2}[f(\mathbf{K}, \mathbf{q}) - f(\mathbf{K}, -\mathbf{q})]$) the integral equation (61) can be written as

$$\left(E - E_0 - \sum_{\boldsymbol{\delta}} [\Delta_1^a(\boldsymbol{\delta}) + \Delta_1^b(\boldsymbol{\delta})] \cos(\mathbf{K} \cdot \boldsymbol{\delta}/\mathbf{2}) \cos(\mathbf{q} \cdot \boldsymbol{\delta}) \right) f(\mathbf{K}, \mathbf{q}) \ =$$

$$\frac{1}{N} \sum_{\mathbf{q}'} f(\mathbf{K}, \mathbf{q}') \sum_{\mathbf{r}, \boldsymbol{\delta_1}, \boldsymbol{\delta_2}} \Delta_2^{ab}(\mathbf{r}, \boldsymbol{\delta_1}, \boldsymbol{\delta_2}) \cos(\mathbf{K} \cdot \mathbf{r}) \sin(\mathbf{q} \cdot \boldsymbol{\delta_1}) \sin(\mathbf{q}' \cdot \boldsymbol{\delta_2}) \ . \quad (68)$$

Identical particles

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If the particles a and b are identical, the solution is the same as for symmetric states except that the labels a and b can now be dropped. However, to avoid double counting it turns out that the Δ_2 term must be adjusted by an extra factor $1/2$:

$$\left(E - E_0 - 2 \sum_{\boldsymbol{\delta}} \Delta_1(\boldsymbol{\delta}) \cos(\mathbf{K} \cdot \boldsymbol{\delta}/2) \cos(\mathbf{q} \cdot \boldsymbol{\delta}) \right) f(\mathbf{K}, \mathbf{q}) =$$

$$\frac{1}{N} \sum_{\mathbf{q}'} f(\mathbf{K}, \mathbf{q}') \left(\frac{1}{2} \sum_{\mathbf{r}, \boldsymbol{\delta_1}, \boldsymbol{\delta_2}} \Delta_2(\mathbf{r}, \boldsymbol{\delta_1}, \boldsymbol{\delta_2}) \cos(\mathbf{K} \cdot \mathbf{r}) \cos(\mathbf{q} \cdot \boldsymbol{\delta_1}) \cos(\mathbf{q}' \cdot \boldsymbol{\delta_2}) \right.$$

$$\left. - 2 \sum_{\boldsymbol{\delta}} \Delta_1(\boldsymbol{\delta}) \cos(\mathbf{K} \cdot \boldsymbol{\delta}/2) \cos(\mathbf{q} \cdot \boldsymbol{\delta}) \right) . \quad (69)$$

Solving the integral equation

The above integral equations can be solved, for a given value of $\mathbf{K}$, using standard discretization techniques. Instead of using the continuous momentum $\mathbf{q}$, one can use N discretized and equally spaced values of momentum. This way one only needs to compute the eigenvalue and eigenvector of an $N \times N$ matrix for the discretized system. Although the matrix is non-symmetric due to the artificially introduced f_{ii} term in Eq. (55), the eigenvalues obtained from this matrix are real. The solutions of the integral equation include an unphysical one with eigenvalue equal to 0 which is ascribed to the unphysical f_{ii} terms. As $N \to \infty$ the results obtained from the calculation with discretized momenta will converge to those with continuous momentum. Actually for those bound states with finite coherence length, the calculation will normally be well converged for quite small values of N, but for unbound states, we have an infinite coherence length, so one may need to do finite N extrapolations to get results at $N = \infty$.

The eigenvalues of the discretized $N \times N$ matrix can be evaluated by using standard numerical techniques. Nevertheless, this approach is restricted to calculate eigenvalues for fixed values of the coupling constant λ and momentum $\mathbf{K}$. That is, we perform a naive sum for the series of Δ_1 and Δ_2. Since we do not obtain explicit series for the energies we can not benefit from using series extrapolation techniques. As a consequence, one may not be able to reach a region of critical coupling.

Analyzing the solutions of the integral equation one generally finds a two-particle continuum which is delimited by the maximum (minimum) energy of two

single particle excitations whose combined momentum is the center of mass momentum. Apart from the unphysical eigenvalue, there may be multiple solutions above or below the two-particle continuum. Those solutions with energy below the bottom edge of the continuum are bound states, while the solutions with energy higher than the upper edge of the continuum are called antibound states. The binding energy is defined as the energy difference between the lower edge of the continuum and the energy of the bound state, while the antibinding energy is defined as the energy difference between the upper edge of continuum and the energy of the respective antibound state.

Note that the series for Δ_2 may depend on the transformation used to block diagonalize the Hamiltonian. If we compute Δ_2 to order n, the resulting series for the two-particle energy obtained from the above integral equation will have two parts: the part up to order n which is independent of the transformation, and the higher order terms which are incomplete and may be transformation dependent. Further note that the series for Δ_2 need not have any singularities. The singularities, if they exist, arise in the solution of the Schrödinger equation. Thus, our method should be able to explore new bound states separating from the continuum as we vary the momentum $\mathbf{K}$. If we get a numerical solution, rather than a series solution, of the Schrödinger equation, we should also be able to explore new bound states as we increase λ as long as the naive sum to the series converges. Examples of both scenarios are presented in the following chapters.

2.4   Series extrapolation

The perturbative calculations using the cluster expansion method result in a truncated series which usually is a polynom in some variable λ. The series is correct in the limit $\lambda \to 0$, but we have only very limited information about the radius of convergence. Thus, it is a standard way to extrapolate the polynomials by Padé or Dlog-Padé approximants [15].

In general a Padé approximant to some finite series is a rational function

$$f(\lambda) = \frac{p_N(\lambda)}{q_M(\lambda)} \ , \tag{70}$$

where $p_N(\lambda)$ and $q_M(\lambda)$ are polynoms in λ of degree N and M respectively. p_N and q_M are chosen in a way that the coefficients of the Taylor series expansion of f match the coefficients of the approximated series up to the given order.

Given the degree [N/M] of the polynoms p_N and q_M the Padé approximant f is uniquely defined. Evaluating a set of different [N/M]-Padé approximants can give valuable information on the stability of the approximation.

If one assumes that the series obeys a power-law dependency without restricting the exponent, it is more suitable to evaluate Dlog-Padé approximants. Given a series $s(\lambda)$ that contains a power-law dependency of the form

$$s(\lambda) = f(\lambda) \cdot (\lambda - \lambda_c)^\nu \, ,$$

where $f(\lambda)$ is a polynom in λ we differentiate the logarithm of $s(\lambda)$

$$Dlog\, s(\lambda) = \frac{f'(\lambda)}{f(\lambda)} + \frac{\nu}{\lambda - \lambda_c} = \frac{p_N(\lambda)}{q_M(\lambda)} \, .$$

The obtained series is a rational function which can be approximated by Padé approximants $\frac{p_N(\lambda)}{q_M(\lambda)}$. The power-law exponent ν can be evaluated by

$$\nu = res_{\lambda_c} \left(\frac{f'(\lambda)}{f(\lambda)} + \frac{\nu}{\lambda - \lambda_c} \right) = \frac{p_N(\lambda_c)}{q'_M(\lambda_c)} \, , \tag{71}$$

where λ_c is a critical point, that is a pole of the Padé approximant.

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