

BACHELOR THESIS

**CORRELATED INTERACTION MATRIX ELEMENTS
WITHIN THE UNITARY CORRELATION
OPERATOR METHOD**

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INTRODUCTION

The journey of nuclear physics began in 1932, when James Chadwick discovered the neutron [1]. Shortly after, it was conceived that the neutron and the already known proton were the fundamental constituents of the atomic nucleus, and the next goal was to study the interaction of these so-called *nucleons*. Today we know that they are not elementary particles. The underlying theory that describes their substructure is quantum chromodynamics. Here, nucleons are understood as a bound object of three quarks, that is held together by an attractive interaction, mediated by messenger particles called gluons. Although possible in principle, it is not yet feasible to provide a description of the atomic nucleus based on interacting quarks and gluons. Instead, the effective concept of interacting inert nucleons is adopted.

A first breakthrough in describing the nucleon-nucleon interaction was the introduction of the meson theory by Hideki Yukawa in 1935 [2]. According to his theory, the interaction between nucleons is mediated through the interchange of mesons, in analogy to electromagnetism, which is mediated through the interchange of photons. The infinite range of the electromagnetic interaction results from the masslessness of the photon. In contrast to that, the range of the nucleon-nucleon interaction is limited by the non-zero meson mass. The theory automatically meets several symmetry requirements, which in turn can provide the basis to find the operator structure of the interaction [3].

First of all, some general symmetries have to be obeyed, like for instance translational and rotational invariance, which are also obeyed by other interactions like gravitation or electromagnetism. In addition to that, the nucleon-nucleon interaction in particular is required to feature parity invariance. Other interactions, like for example the weak interaction, break this symmetry. Since only a limited set of operators meets these requirements, we can narrow the general operator structure of the nucleon-nucleon interaction. The remaining radial dependencies include parameters that are adjusted to experimental results. Interactions that reproduce deuteron properties and results of nucleon-nucleon scattering in particular are called *realistic nucleon-nucleon interactions*.

Aside from general symmetry considerations, it is possible to take empirical findings into account [3]. The binding energy per nucleon has a typical value of approximately 8 MeV across the entire mass range, which suggests the dominance of the interaction between next neighbors and therewith the overall short range of the nucleon-nucleon interaction. Furthermore, the fact that stable nuclei exist means that there must be an attractive component to the nucleon-nucleon interaction. The average internucleon distance of 1 – 2 fm implicates

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the magnitude of this mid-range attraction. Another important characteristic is a strong repulsion at short distances, which is observed at nucleon-nucleon scattering experiments. Moreover, the non vanishing quadrupole moment of the deuteron shows that its ground state is a superposition of states with different angular momenta. This can only be produced by interactions with non-vanishing matrix elements between states with different angular momenta. The so-called tensor interaction is the simplest of them. Finally, experimental findings such as spin-orbit splitting of nuclear energy levels provide an indication of the contribution of a spin-orbit interaction. The two most important types of correlations between nucleons suggested by empirical evidence are the *central correlations*, generated by the short-range repulsion, and the *tensor correlations*, induced by the short-range component of the tensor interaction.

In essence, there are two different approaches to solve the nuclear many-body problem on this basis. One strategy to do so is by means of numerical calculations, without making any conceptual approximations. The two most prominent of these so-called *ab initio* methods are the No-Core Shell Model (NCSM) and the Green's Function Monte Carlo (GFMC) method. Unfortunately, the enormous computational costs resulting from the complexity of the problem limit the practicability of these methods to nuclei with small mass numbers. Another strategy is to find approximate solutions, of which one group is given by the mean field methods. They are based upon the assumption of non-interacting nucleons, which are immersed in an external one-body potential. This so called mean field potential can be derived from a two-body interaction, as it is done for example in the Hartree-Fock method. However, these methods prove to be incompatible with realistic nucleon-nucleon interactions, because the strong short-range correlations induced by realistic nucleon-nucleon interactions go beyond the concept of non-interacting nucleons.

In the first chapter we will present the Unitary Correlation Operator Method, a concept that resolves this problem by imprinting the dominant short-range central and tensor correlations into a many-body state. On this basis, we will subsequently in the second chapter derive matrix elements of an interaction operator that includes the central and the tensor correlations both in harmonic oscillator and momentum space representation. For our calculations we will use the Argonne v_{18} potential [4], a realistic nucleon-nucleon potential whose corresponding operator can be decomposed into 18 operators. A summary and outlook will be given in the third and final chapter.

CHAPTER 1

THE UNITARY CORRELATION OPERATOR METHOD

As we have described in the introduction, mean field methods for solving the nuclear many-body problem cannot account for the strong short-range correlations induced by realistic nucleon-nucleon interactions. The Unitary Correlation Operator Method (UCOM) provides a solution to this problem [5, 6, 7, 8]. Here, the strong short-range correlations are explicitly described by a state-independent unitary transformation:

$$|\tilde{\Psi}\rangle = C|\Psi\rangle, \quad \text{with } C^\dagger C = \mathbb{1}. \quad (1.1)$$

The correlation operator C maps the uncorrelated state $|\Psi\rangle$ to the correlated state $|\tilde{\Psi}\rangle$, which incorporates the strong short-range correlations. Matrix elements with correlated states of an operator O are equivalent to matrix elements with uncorrelated states of a corresponding correlated operator \tilde{O} :

$$\langle \tilde{\Psi} | O | \tilde{\Psi}' \rangle = \langle \Psi | C^\dagger O C | \Psi' \rangle = \langle \Psi | \tilde{O} | \Psi' \rangle. \quad (1.2)$$

The correlated operator is defined by equation (1.2). The unitarity of C leads to

$$\tilde{O} = C^\dagger O C = C^{-1} O C. \quad (1.3)$$

We construct the correlation operator to comprise the two dominant components of the short-range correlations, the repulsion of the central interaction and the contribution of the tensor interaction. For convenience we split the correlation operator into two unitary operators C_r and C_Ω that describe the different types of correlations:

$$C = C_\Omega C_r, \quad (1.4)$$

where C_Ω denotes the tensor correlator and C_r the central correlator. In order to ensure their unitarity, they are written as exponentials of hermitian generators G_i , where i represents

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either r or Ω :

$$C_i = \exp\{-iG_i\} , \quad \text{with } G_i = G_i^\dagger . \quad (1.5)$$

For systems with small densities, the correlations are in good approximation two-body correlations, which means that we can express the hermitian generators in terms of two-body operators:

$$G_i = \sum_{m<n} g_i^{(mn)} . \quad (1.6)$$

Consequently, the correlation operators read

$$C_r = \exp\{-i \sum_{m<n} g_r^{(mn)}\} , \quad (1.7)$$

$$C_\Omega = \exp\{-i \sum_{m<n} g_\Omega^{(mn)}\} . \quad (1.8)$$

In the following sections we will discuss both the central and the tensor correlations.

1.1 Central Correlations

The short-range repulsion of the central interaction prevents two nucleons from moving too close together. To this end, the central correlator is required to move apart two nucleons in radial direction, depending on their relative distance. Radial shifts are generated by the projection of the relative momentum $\mathbf{q} = \frac{1}{2}(\mathbf{p}_1 - \mathbf{p}_2)$ onto the relative distance vector $\mathbf{r} = \mathbf{x}_1 - \mathbf{x}_2$, called *radial momentum*:

$$q_r = \frac{1}{2} \left(\mathbf{q} \cdot \frac{\mathbf{r}}{r} + \frac{\mathbf{r}}{r} \cdot \mathbf{q} \right) . \quad (1.9)$$

The radial shifts have to be large at small distances and subside at large distances. This distance dependence is described by the shift function $s(r)$. Thus, the generator of the central correlations is given by

$$g_r = \frac{1}{2} \left(s(r) q_r + q_r s(r) \right) . \quad (1.10)$$

Next we consider the effect of the central correlator on a two-nucleon state $|\Psi\rangle = |\Psi_{\text{cm}}\rangle \otimes |\Phi\rangle$, which we separate into a center of mass and a relative component. Since the central correlator only depends on relative coordinates, it has no effect on the center of mass component $|\Psi_{\text{cm}}\rangle$. For the relative component $|\Phi\rangle$ we assume *LS*-coupled angular momentum eigenstates $|\phi(LS)JMTM_T\rangle$. To simplify matters, we omit the projection quantum numbers M and M_T in the following. According to equation (1.7), the central correlator for a

two-nucleon system is given by $c_r = \exp\{-ig_r\}$.

In coordinate representation, the centrally correlated states are given by [9]

$$\langle r|c_r|\phi\rangle = \mathcal{R}_-(r) \langle R_-(r)|\phi\rangle , \quad (1.11)$$

$$\langle r|c_r^\dagger|\phi\rangle = \mathcal{R}_+(r) \langle R_+(r)|\phi\rangle , \quad (1.12)$$

using the definition

$$\mathcal{R}_\pm(r) = \frac{R_\pm(r)}{r} \sqrt{\frac{\partial R_\pm(r)}{\partial r}} . \quad (1.13)$$

We note that only the radial component $|\phi\rangle$ is affected, while the angular momentum and spin components remain unchanged. The mutually inverse functions $R_\pm(r)$ are called correlation functions, and are related to the shift function $s(r)$ through

$$\int_r^{R_\pm(r)} \frac{d\xi}{s(\xi)} = \pm 1 . \quad (1.14)$$

By approximation we obtain $R_\pm(r) \approx r \pm s(r)$, implying that in equation (1.11) the two nucleons are moved apart by $s(r)$, if they were previously separated by r .

Furthermore, we note that the similarity transformation of the relative distance operator is given by [9]

$$c_r^\dagger r c_r = R_+(r) . \quad (1.15)$$

The unitarity of c_r implies that an arbitrary function $f(r)$ transforms as

$$c_r^\dagger f(r) c_r = f(c_r^\dagger r c_r) = f(R_+(r)) , \quad (1.16)$$

as can be inferred from its power series representation.

1.2 Tensor Correlations

The tensor interaction induces correlations between the spins σ_1 and σ_2 of two nucleons with their relative distance vector \mathbf{r} [3]. The tensor correlator is required to shift the nucleons transversal to their relative distance vector, depending on the relative orientation and distance of the two spins. Transversal shifts are generated by the difference between the relative momentum and its radial component, called *orbital momentum*:

$$\mathbf{q}_\Omega = \mathbf{q} - \frac{\mathbf{r}}{r} q_r = \frac{1}{2} \left(\mathbf{1} \times \frac{\mathbf{r}}{r} - \frac{\mathbf{r}}{r} \times \mathbf{1} \right) , \quad (1.17)$$

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where $\mathbf{l} = \mathbf{r} \times \mathbf{q}$ denotes the orbital angular momentum. Analogous to $s(r)$, the distance dependence of the transversal shifts is described by the tensor correlation function $\vartheta(r)$. On this basis, the generator of the tensor correlations is constructed:

$$\mathbf{g}_\Omega = \vartheta(r) \frac{3}{2} \left((\boldsymbol{\sigma}_1 \cdot \mathbf{r})(\boldsymbol{\sigma}_2 \cdot \mathbf{q}_\Omega) + (\boldsymbol{\sigma}_1 \cdot \mathbf{q}_\Omega)(\boldsymbol{\sigma}_2 \cdot \mathbf{r}) \right) = \vartheta(r) s_{12}(\mathbf{r}, \mathbf{q}_\Omega) , \quad (1.18)$$

where s_{12} denotes the general tensor operator

$$s_{12}(\mathbf{a}, \mathbf{b}) = \frac{3}{2} \left((\boldsymbol{\sigma}_1 \cdot \mathbf{a})(\boldsymbol{\sigma}_2 \cdot \mathbf{b}) + (\boldsymbol{\sigma}_1 \cdot \mathbf{b})(\boldsymbol{\sigma}_2 \cdot \mathbf{a}) \right) - \frac{1}{2} (\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2) (\mathbf{a} \cdot \mathbf{b} + \mathbf{b} \cdot \mathbf{a}) . \quad (1.19)$$

Next we consider the effect of the tensor correlator on a two-nucleon state [9]. As in the case of the central correlator, the center of mass component is invariant under the transformation, since the tensor correlator only depends on relative coordinates. Again, we assume LS -coupled angular momentum eigenstates $|\phi(LS)JT\rangle$ for the relative component. According to equation (1.8), the tensor correlator for a two-nucleon system is given by $c_\Omega = \exp\{-i\mathbf{g}_\Omega\}$. To find relations for the tensor correlated two-nucleon states, we first ascertain their possible angular momenta. Since they have to be antisymmetric, $L+S+T$ must give an odd number [3]. Furthermore, angular momentum coupling requires $|L-S| \leq J \leq L+S$. As a result, L can only take values J or $J \pm 1$ for $S = 1$, and only J for $S = 0$. Consequently, $L = J$ and $L = J \pm 1$ are the only possibilities we have to analyze in general. We now consider the non-zero matrix elements of the tensor operator [8]:

$$\langle \phi(J \pm 1, 1)JT | s_{12}(\mathbf{r}, \mathbf{q}_\Omega) | \phi(J \mp 1, 1)JT \rangle = \pm 3i \sqrt{J(J+1)} . \quad (1.20)$$

Combining equations (1.18) and (1.20) yields the non-zero matrix elements of $-i\mathbf{g}_\Omega$:

$$\langle \phi(J \pm 1, 1)JT | -i\mathbf{g}_\Omega | \phi(J \mp 1, 1)JT \rangle = \pm \theta_J(r) , \quad (1.21)$$

where we have used the definition

$$\theta_J(r) = 3\sqrt{J(J+1)} \vartheta(r) . \quad (1.22)$$

By evaluating the corresponding matrix exponential we find the matrix elements of the tensor correlator:

c_Ω	$ \phi(J-1, 1)JT\rangle$	$ \phi(JS)JT\rangle$	$ \phi(J+1, 1)JT\rangle$
$\langle \phi(J-1, 1)JT $	$\cos \theta_J(r)$	0	$-\sin \theta_J(r)$
$\langle \phi(JS)JT $	0	1	0
$\langle \phi(J+1, 1)JT $	$\sin \theta_J(r)$	0	$\cos \theta_J(r)$

From this we can directly read off explicit relations for the tensor correlated states.

For $L = J$ the states are invariant under the transformation

$$c_\Omega |\phi(JS)JT\rangle = |\phi(JS)JT\rangle , \quad (1.23)$$

while states with $L = J \pm 1$ transform like

$$c_{\Omega} |\phi(J \pm 1, 1)JT\rangle = \cos \theta_J(r) |\phi(J \pm 1, 1)JT\rangle \mp \sin \theta_J(r) |\phi(J \mp 1, 1)JT\rangle . \quad (1.24)$$

Similarly, for the adjoint tensor correlator $c_{\Omega}^{\dagger} = \exp\{i\mathbf{g}_{\Omega}\}$ we find that states with $L = J$ are invariant

$$c_{\Omega}^{\dagger} |\phi(JS)JT\rangle = |\phi(JS)JT\rangle , \quad (1.25)$$

while states with $L = J \pm 1$ transform like

$$c_{\Omega}^{\dagger} |\phi(J \pm 1, 1)JT\rangle = \cos \theta_J(r) |\phi(J \pm 1, 1)JT\rangle \pm \sin \theta_J(r) |\phi(J \mp 1, 1)JT\rangle . \quad (1.26)$$

1.3 Spin-Isospin Dependence

The nucleon-nucleon interaction can be projected onto the different spin-isospin channels [10]. This proves to be useful, since certain parts of the interaction do not contribute in all of them. In particular, the tensor and spin-orbit components only have contributions in the $S = 1$ channels. Accordingly, we can write the generators in general as

$$\mathbf{g}_i = \sum_{ST} \mathbf{g}_{i,ST} \Pi_{ST} , \quad (1.27)$$

where i represents either r or Ω and where Π_{ST} denotes the projection operator onto spin and isospin. On this note, the generators of the central and the tensor correlations can be written as

$$\mathbf{g}_r = \sum_{S,T} \frac{1}{2} \left(s_{ST}(r) \mathbf{q}_r + \mathbf{q}_r s_{ST}(r) \right) \Pi_{ST} , \quad (1.28)$$

$$\mathbf{g}_{\Omega} = \sum_T \vartheta_T(r) s_{12}(\mathbf{r}, \mathbf{q}_{\Omega}) \Pi_{1T} , \quad (1.29)$$

where $s_{ST}(r)$ and $\vartheta_T(r)$ denote the shift function and the tensor correlation function for each spin-isospin channel. For the correlators in a two-nucleon system, equation (1.27) yields

$$c_i = \exp\{-i\mathbf{g}_i\} = \exp\{-i \sum_{ST} \mathbf{g}_{i,ST} \Pi_{ST}\} = \sum_{ST} \exp\{-i\mathbf{g}_{i,ST}\} \Pi_{ST} = \sum_{ST} c_{ST} \Pi_{ST} , \quad (1.30)$$

implying that the correlators can be determined independently for the different spin-isospin channels.

1.4 Cluster Expansion

A correlated operator generated by the unitarity transformation (1.3) can be expanded into a series of irreducible contributions to all particle numbers [5]:

$$\tilde{O} = C^\dagger O C = \sum_{n=1}^{\infty} \tilde{O}^{[n]} , \quad (1.31)$$

where $\tilde{O}^{[n]}$ denotes the irreducible n -body contribution. Equation (1.31) is called a cluster expansion. If O is a k -body operator, all irreducible contributions with $n < k$ vanish. Provided the range of the correlation functions is small compared to the mean interparticle distance, we can make use of the two-body approximation

$$\tilde{O}^{C2} = \tilde{O}^{[1]} + \tilde{O}^{[2]} , \quad (1.32)$$

where three-body and higher-order contributions are neglected. In principle, all contributions to the cluster expansion can be evaluated [11]. However, for many-body calculations their inclusion is an extreme challenge. Since we will only deal with two-body problems in this work, equation (1.32) provides an exact description.

CHAPTER 2

CORRELATED INTERACTION

Having introduced the Unitary Correlation Operator Method, we can now study the matrix elements of the correlated interaction operator $\tilde{v} = c^\dagger v c$ for a two-nucleon system in both harmonic oscillator and momentum space representation. As indicated in sections 1.1 and 1.2, we consider LS -coupled angular momentum eigenstates $|\phi(LS)JT\rangle$ for the relative component of the two-nucleon state. In order to obtain the matrix elements of \tilde{v} , we first have to derive the matrix elements of the correlation operator $c = c_\Omega c_r$.

2.1 Harmonic Oscillator Representation

In harmonic oscillator representation, the radial wave function ϕ is represented by a generic radial quantum number n . The relative wave functions are given by the harmonic oscillator eigenfunctions:

$$\langle r(LS)JT | n(LS)JT \rangle = N_{nL} r^L e^{-\nu r^2} \mathcal{L}_n^{L+1/2}(2\nu r^2), \quad (2.1)$$

using the definitions

$$N_{nL} = \sqrt{\sqrt{\frac{2\nu^3}{\pi}} \frac{2^{n+2L+3} n! \nu^L}{(2n+2L+1)!!}}, \quad \nu = \frac{\mu\omega}{2}, \quad (2.2)$$

where μ denotes the reduced mass and ω the frequency of the harmonic oscillator. Here and in the following, we employ a system of units with $\hbar = 1$. For our calculations we assume $\nu = 0.12 \text{ fm}^{-2}$, which corresponds to $\hbar\omega = 20 \text{ MeV}$. The generalized Laguerre polynomials are given by

$$\mathcal{L}_n^k(x) = \sum_{i=0}^n \binom{n+k}{n-i} \frac{(-x)^i}{i!}. \quad (2.3)$$

2 Correlated Interaction

2.1.1 Correlation Operator Matrix Elements

Using the formal framework of the harmonic oscillator representation, we can derive the corresponding matrix elements of the correlation operator:

$$\begin{aligned}
& \langle n(LS)JT | c_{\Omega} c_r | n'(L'S)JT \rangle \\
&= \sum_{L''S''J''T''} \int dr r^2 \langle n(LS)JT | r(L''S'')J''T'' \rangle \langle r(L''S'')J''T'' | c_{\Omega} c_r | n'(L'S)JT \rangle \\
&= \int dr r^2 \langle n(LS)JT | r(LS)JT \rangle \langle r(LS)JT | c_{\Omega} c_r | n'(L'S)JT \rangle ,
\end{aligned} \tag{2.4}$$

where we have inserted the identity operator in position space representation and subsequently used the orthogonality of the harmonic oscillator eigenfunctions. For L and L' we distinguish three cases.

For $L = L' = J$ we find:

$$\begin{aligned}
& \langle n(JS)JT | c_{\Omega} c_r | n'(JS)JT \rangle \\
&\stackrel{(2.4)}{=} \int dr r^2 \langle n(JS)JT | r(JS)JT \rangle \langle r(JS)JT | c_{\Omega} c_r | n'(JS)JT \rangle .
\end{aligned}$$

According to equation (1.25), the tensor correlator does not have an effect here:

$$= \int dr r^2 \langle n(JS)JT | r(JS)JT \rangle \langle r(JS)JT | c_r | n'(JS)JT \rangle .$$

Using equation (1.11) we evaluate the transformation of the central correlator:

$$= \int dr r^2 \mathcal{R}_-(r) \langle n(JS)JT | r(JS)JT \rangle \langle R_-(r) (JS)JT | n'(JS)JT \rangle .$$

Analogous, for $L = L' = J \pm 1$ we find

$$\begin{aligned}
& \langle n(J \pm 1, 1)JT | c_{\Omega} c_r | n'(J \pm 1, 1)JT \rangle \\
&\stackrel{(2.4)}{=} \int dr r^2 \langle n(J \pm 1, 1)JT | r(J \pm 1, 1)JT \rangle \langle r(J \pm 1, 1)JT | c_{\Omega} c_r | n'(J \pm 1, 1)JT \rangle .
\end{aligned}$$

2.1 Harmonic Oscillator Representation

Here we use equation (1.26) to evaluate the transformation of the tensor correlator:

$$\begin{aligned}
&= \int dr r^2 \langle n(J \pm 1, 1)JT | r(J \pm 1, 1)JT \rangle \\
&\quad \times \left(\langle r(J \pm 1, 1)JT | \cos \theta_J(\mathbf{r}) c_r | n'(J \pm 1, 1)JT \rangle \right. \\
&\quad \left. \pm \langle r(J \mp 1, 1)JT | \sin \theta_J(\mathbf{r}) c_r | n'(J \pm 1, 1)JT \rangle \right) .
\end{aligned}$$

Inserting the identity operator $c_r c_r^\dagger$ leads to an expression that can be evaluated using equation (1.16):

$$\begin{aligned}
&= \int dr r^2 \langle n(J \pm 1, 1)JT | r(J \pm 1, 1)JT \rangle \\
&\quad \times \left(\langle r(J \pm 1, 1)JT | c_r c_r^\dagger \cos \theta_J(\mathbf{r}) c_r | n'(J \pm 1, 1)JT \rangle \right. \\
&\quad \left. \pm \langle r(J \mp 1, 1)JT | c_r c_r^\dagger \sin \theta_J(\mathbf{r}) c_r | n'(J \pm 1, 1)JT \rangle \right) \\
&= \int dr r^2 \langle n(J \pm 1, 1)JT | r(J \pm 1, 1)JT \rangle \\
&\quad \times \left(\langle r(J \pm 1, 1)JT | c_r \cos \theta_J(R_+(\mathbf{r})) | n'(J \pm 1, 1)JT \rangle \right. \\
&\quad \left. \pm \langle r(J \mp 1, 1)JT | c_r \sin \theta_J(R_+(\mathbf{r})) | n'(J \pm 1, 1)JT \rangle \right) .
\end{aligned}$$

Making use of equation (1.11), we evaluate the transformation of the central correlator:

$$\begin{aligned}
&= \int dr r^2 \langle n(J \pm 1, 1)JT | r(J \pm 1, 1)JT \rangle \mathcal{R}_-(r) \\
&\quad \times \left(\cos \theta_J(R_+(r)) \langle R_-(r)(J \pm 1, 1)JT | n'(J \pm 1, 1)JT \rangle \right. \\
&\quad \left. \pm \sin \theta_J(R_+(r)) \langle R_-(r)(J \mp 1, 1)JT | n'(J \pm 1, 1)JT \rangle \right) .
\end{aligned}$$

Since the harmonic oscillator eigenfunctions are orthonormal, we get

$$\begin{aligned}
&= \int dr r^2 \langle n(J \pm 1, 1)JT | r(J \pm 1, 1)JT \rangle \mathcal{R}_-(r) \\
&\quad \times \cos \theta_J(R_+(r)) \langle R_-(r)(J \pm 1, 1)JT | n'(J \pm 1, 1)JT \rangle .
\end{aligned}$$

Finally, for $L = J \pm 1$ and $L' = J \mp 1$ we find

$$\begin{aligned}
&\langle n(J \pm 1, 1)JT | c_\Omega c_r | n'(J \mp 1, 1)JT \rangle \\
&\stackrel{(2.4)}{=} \int dr r^2 \langle n(J \pm 1, 1)JT | r(J \pm 1, 1)JT \rangle \langle r(J \pm 1, 1)JT | c_\Omega c_r | n'(J \mp 1, 1)JT \rangle .
\end{aligned}$$

2 Correlated Interaction

Again we use equation (1.26) to evaluate the transformation of the tensor correlator:

$$\begin{aligned}
&= \int dr r^2 \langle n(J \pm 1, 1)JT | r(J \pm 1, 1)JT \rangle \\
&\quad \times \left(\langle r(J \pm 1, 1)JT | \cos \theta_J(r) c_r | n'(J \mp 1, 1)JT \rangle \right. \\
&\quad \left. \pm \langle r(J \mp 1, 1)JT | \sin \theta_J(r) c_r | n'(J \mp 1, 1)JT \rangle \right) .
\end{aligned}$$

As before, inserting the identity operator $c_r c_r^\dagger$ leads to an expression that can be evaluated using equation (1.16):

$$\begin{aligned}
&= \int dr r^2 \langle n(J \pm 1, 1)JT | r(J \pm 1, 1)JT \rangle \\
&\quad \times \left(\langle r(J \pm 1, 1)JT | c_r c_r^\dagger \cos \theta_J(r) c_r | n'(J \mp 1, 1)JT \rangle \right. \\
&\quad \left. \pm \langle r(J \mp 1, 1)JT | c_r c_r^\dagger \sin \theta_J(r) c_r | n'(J \mp 1, 1)JT \rangle \right) \\
&= \int dr r^2 \langle n(J \pm 1, 1)JT | r(J \pm 1, 1)JT \rangle \\
&\quad \times \left(\langle r(J \pm 1, 1)JT | c_r \cos \theta_J(R_+(r)) | n'(J \mp 1, 1)JT \rangle \right. \\
&\quad \left. \pm \langle r(J \mp 1, 1)JT | c_r \sin \theta_J(R_+(r)) | n'(J \mp 1, 1)JT \rangle \right) .
\end{aligned}$$

With equation (1.11) we evaluate the transformation of the central correlator:

$$\begin{aligned}
&= \int dr r^2 \langle n(J \pm 1, 1)JT | r(J \pm 1, 1)JT \rangle \mathcal{R}_-(r) \\
&\quad \times \left(\cos \theta_J(R_+(r)) \langle R_-(r)(J \pm 1, 1)JT | n'(J \mp 1, 1)JT \rangle \right. \\
&\quad \left. \pm \sin \theta_J(R_+(r)) \langle R_-(r)(J \mp 1, 1)JT | n'(J \mp 1, 1)JT \rangle \right) .
\end{aligned}$$

The orthonormality of the harmonic oscillator eigenfunctions leads to

$$\begin{aligned}
&= \pm \int dr r^2 \langle n(J \pm 1, 1)JT | r(J \pm 1, 1)JT \rangle \mathcal{R}_-(r) \\
&\quad \times \sin \theta_J(R_+(r)) \langle R_-(r)(J \mp 1, 1)JT | n'(J \mp 1, 1)JT \rangle .
\end{aligned}$$

For the sake of clarity, the resulting non-zero matrix elements $\langle n(LS)JT | c_\Omega c_r | n'(L'S)JT \rangle$ for

all combinations of L and L' are listed below.

$$\begin{aligned}
 \langle n(JS)JT | c_{\Omega} c_r | n'(JS)JT \rangle &= \int dr r^2 \mathcal{R}_-(r) \langle r(JS)JT | n(JS)JT \rangle^* \\
 &\quad \times \langle R_-(r)(JS)JT | n'(JS)JT \rangle \\
 \langle n(J \pm 1, 1)JT | c_{\Omega} c_r | n'(J \pm 1, 1)JT \rangle &= \int dr r^2 \mathcal{R}_-(r) \langle r(J \pm 1, 1)JT | n(J \pm 1, 1)JT \rangle^* \\
 &\quad \times \cos \theta_J(R_+(r)) \langle R_-(r)(J \pm 1, 1)JT | n'(J \pm 1, 1)JT \rangle \\
 \langle n(J \pm 1, 1)JT | c_{\Omega} c_r | n'(J \mp 1, 1)JT \rangle &= \pm \int dr r^2 \mathcal{R}_-(r) \langle r(J \pm 1, 1)JT | n(J \pm 1, 1)JT \rangle^* \\
 &\quad \times \sin \theta_J(R_+(r)) \langle R_-(r)(J \mp 1, 1)JT | n'(J \mp 1, 1)JT \rangle .
 \end{aligned} \tag{2.5}$$

For some specific partial waves, the resulting matrices for all possible combinations of L and L' are illustrated in figures 2.1 and 2.2. We observe that all matrices with $L = L'$ share a similar structure. As a result of normalization, their main diagonal elements are approximately equal to unity. Furthermore, the matrices with $L \neq L'$ share a similar structure as well. Overall, we notice significant off-diagonal contributions in all cases.

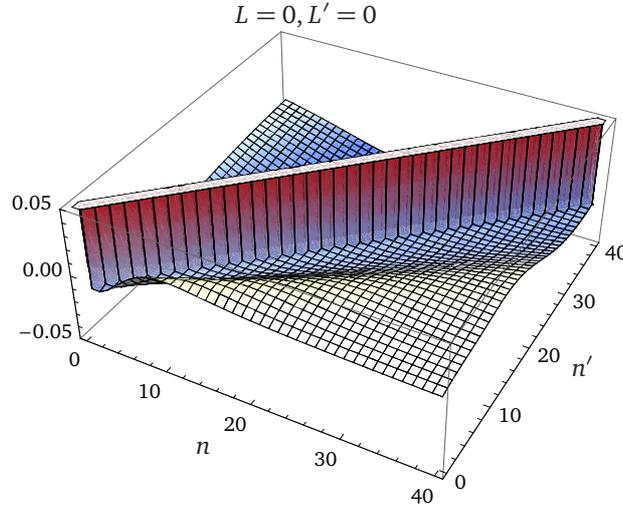


Figure 2.1: Correlation operator matrix elements for $J = 0$, $S = 0$ and $T = 1$ for the only possible combination of L and L'

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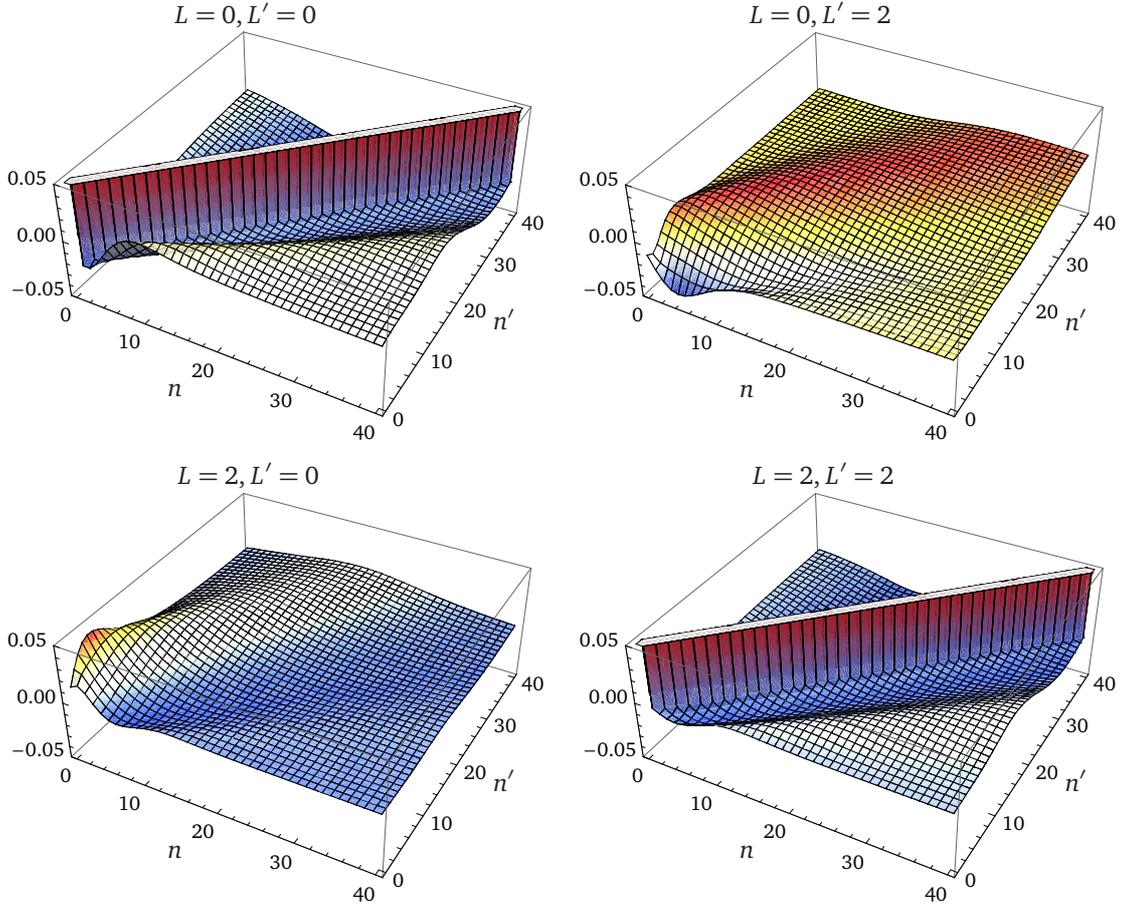


Figure 2.2: Correlation operator matrix elements for $J = 1$, $S = 1$ and $T = 0$ for all possible combinations of L and L'

2.1.2 Verification of Unitarity

In this section, we want to validate our numerical calculations and assess the applicability of our results. Due to the unitarity of the correlation operator c , we expect the norm of any state to be preserved under the transformation. Considering that the harmonic oscillator eigenstates $|n(LS)JT\rangle$ are mutually orthonormal, we have to verify that

$$\langle n(LS)JT | c^\dagger c | n'(L'S)JT \rangle \stackrel{!}{=} \langle n(LS)JT | n'(L'S)JT \rangle = \delta_{nn'} \delta_{LL'} \quad (2.6)$$

is satisfied. To this end, we express the matrix elements of $c^\dagger c$ in terms of the matrix elements listed above in (2.5) by inserting the identity operator in harmonic oscillator representation

and obtain

$$\begin{aligned}
 & \langle n(LS)JT | c^\dagger c | n'(L'S)JT \rangle \\
 &= \sum_{n''L''} \langle n(LS)JT | c^\dagger | n''(L''S)JT \rangle \langle n''(L''S)JT | c | n'(L'S)JT \rangle \\
 &= \sum_{n''L''} \langle n''(L''S)JT | c | n(LS)JT \rangle^* \langle n''(L''S)JT | c | n'(L'S)JT \rangle .
 \end{aligned} \tag{2.7}$$

Here, we distinguish three cases. For $L = L' = J$ we find

$$\begin{aligned}
 & \langle n(JS)JT | c^\dagger c | n'(JS)JT \rangle \\
 &\stackrel{(2.7)}{=} \sum_{n''L''} \langle n''(L''S)JT | c | n(JS)JT \rangle^* \langle n''(L''S)JT | c | n'(JS)JT \rangle \\
 &\stackrel{(2.5)}{=} \sum_{n''} \langle n''(JS)JT | c | n(JS)JT \rangle^* \langle n''(JS)JT | c | n'(JS)JT \rangle .
 \end{aligned} \tag{2.8}$$

Analogous, for $L = L' = J \pm 1$ we find

$$\begin{aligned}
 & \langle n(J \pm 1, 1)JT | c^\dagger c | n'(J \pm 1, 1)JT \rangle \\
 &\stackrel{(2.7)}{=} \sum_{n''L''} \langle n''(L''S)JT | c | n(J \pm 1, 1)JT \rangle^* \langle n''(L''S)JT | c | n'(J \pm 1, 1)JT \rangle \\
 &\stackrel{(2.5)}{=} \sum_{n''} \left(\langle n''(J + 1, 1)JT | c | n(J \pm 1, 1)JT \rangle^* \langle n''(J + 1, 1)JT | c | n'(J \pm 1, 1)JT \rangle \right. \\
 &\quad \left. + \langle n''(J - 1, 1)JT | c | n(J \pm 1, 1)JT \rangle^* \langle n''(J - 1, 1)JT | c | n'(J \pm 1, 1)JT \rangle \right) .
 \end{aligned} \tag{2.9}$$

And for $L = J \pm 1$ and $L' = J \mp 1$ we find

$$\begin{aligned}
 & \langle n(J \pm 1, 1)JT | c^\dagger c | n'(J \mp 1, 1)JT \rangle \\
 &\stackrel{(2.7)}{=} \sum_{n''L''} \langle n''(L''S)JT | c | n(J \pm 1, 1)JT \rangle^* \langle n''(L''S)JT | c | n'(J \mp 1, 1)JT \rangle \\
 &\stackrel{(2.5)}{=} \sum_{n''} \left(\langle n''(J + 1, 1)JT | c | n(J \pm 1, 1)JT \rangle^* \langle n''(J + 1, 1)JT | c | n'(J \mp 1, 1)JT \rangle \right. \\
 &\quad \left. + \langle n''(J - 1, 1)JT | c | n(J \pm 1, 1)JT \rangle^* \langle n''(J - 1, 1)JT | c | n'(J \mp 1, 1)JT \rangle \right) .
 \end{aligned} \tag{2.10}$$

In order to evaluate the matrix elements $\langle n(LS)JT | c^\dagger c | n'(L'S)JT \rangle$ numerically, it is necessary to truncate the summation over n'' . Due to the large off-diagonal contributions of the correlation operator matrix mentioned before, the impact of truncation is more significant for large quantum numbers n and n' . Consequently, we expect unitarity to be satisfied well for small quantum numbers n and n' only. For the same specific partial waves as in the previous section, the matrices corresponding to the matrix elements $\delta_{nn'} \delta_{LL'} - \langle n(LS)JT | c^\dagger c | n'(L'S)JT \rangle$ are illustrated in figures 2.3 and 2.4 for all possible combinations of L and L' . In accor-

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dance with equation (2.6), all matrices equal the zero matrix in good approximation for small quantum numbers n and n' , while for large n and n' there are substantial deviations as expected.

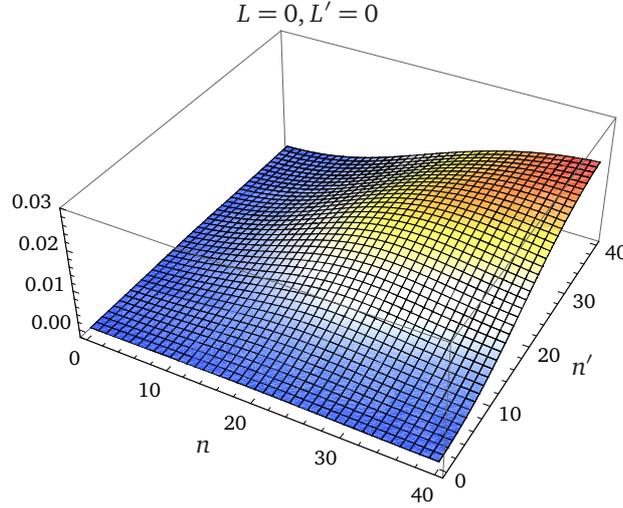


Figure 2.3: Unitarity verification for $J = 0$, $S = 0$ and $T = 1$ for the only possible combination of L and L'

2.1.3 Correlated Interaction Matrix Elements

Starting from the matrix elements of the uncorrelated interaction operator v , we can now calculate the matrix elements of the correlated interaction operator \tilde{v} with the results of the previous sections. According to equation (1.3) we get

$$\begin{aligned}
 & \langle n(LS)JT | \tilde{v} | n'(L'S)JT \rangle \\
 &= \langle n(LS)JT | c^\dagger v c | n'(L'S)JT \rangle \\
 &= \sum_{n''L''} \sum_{n'''L'''} \langle n(LS)JT | c^\dagger | n''(L''S)JT \rangle \langle n''(L''S)JT | v | n'''(L'''S)JT \rangle \\
 & \quad \times \langle n'''(L'''S)JT | c | n'(L'S)JT \rangle \\
 &= \sum_{n''L''} \sum_{n'''L'''} \langle n''(L''S)JT | c | n(LS)JT \rangle^* \langle n''(L''S)JT | v | n'''(L'''S)JT \rangle \\
 & \quad \times \langle n'''(L'''S)JT | c | n'(L'S)JT \rangle ,
 \end{aligned} \tag{2.11}$$

where we have inserted two identity operators in harmonic oscillator representation. Using equation (2.5), we can evaluate this sum. Again, we distinguish three cases. For $L = L' = J$

2.1 Harmonic Oscillator Representation

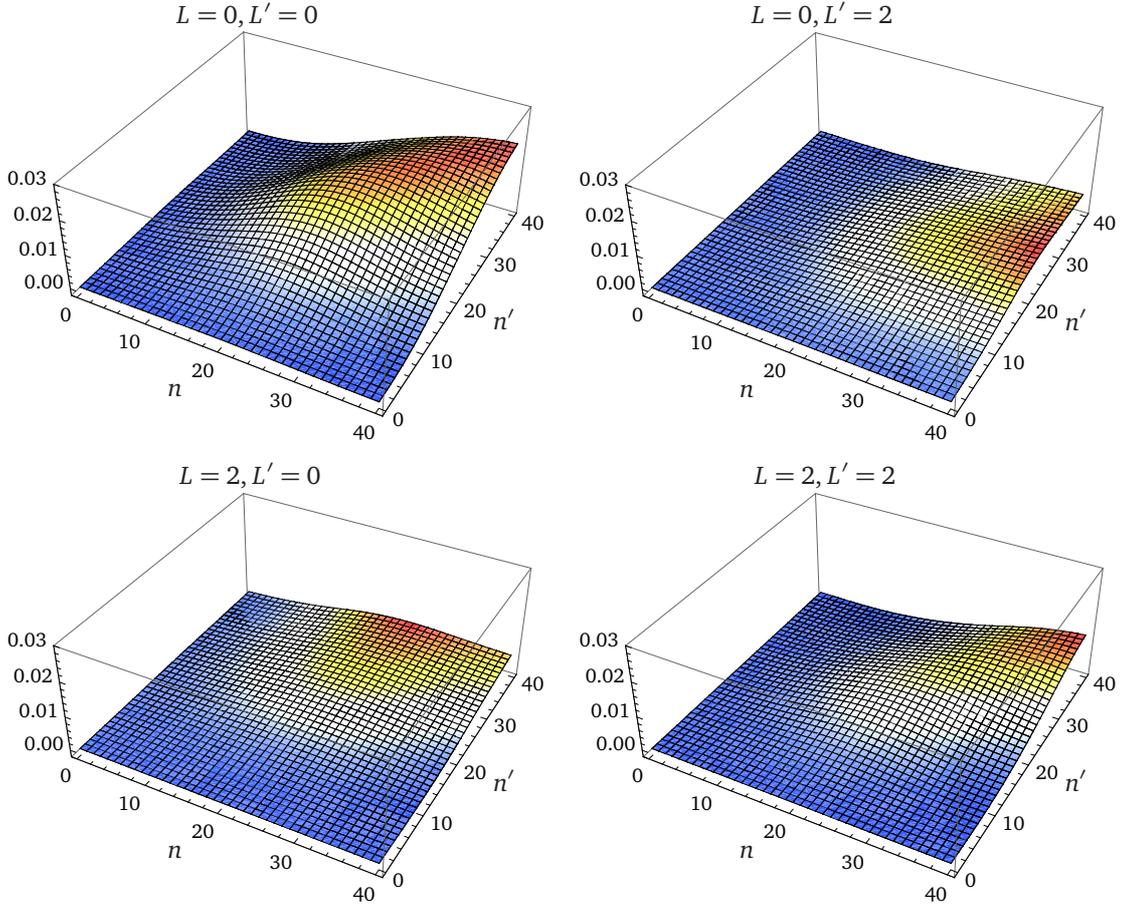


Figure 2.4: Unitarity verification for $J = 1$, $S = 1$ and $T = 0$ for all possible combinations of L and L'

we find

$$\begin{aligned}
 & \langle n(JS)JT | \tilde{v} | n'(JS)JT \rangle \\
 & \stackrel{(2.11)}{=} \sum_{n''L''} \sum_{n'''L'''} \langle n''(L''S)JT | c | n(JS)JT \rangle^* \langle n''(L''S)JT | v | n'''(L'''S)JT \rangle \\
 & \quad \times \langle n'''(L'''S)JT | c | n'(JS)JT \rangle \tag{2.12} \\
 & \stackrel{(2.5)}{=} \sum_{n''} \sum_{n'''} \langle n''(JS)JT | c | n(JS)JT \rangle^* \langle n''(JS)JT | v | n'''(JS)JT \rangle \\
 & \quad \times \langle n'''(JS)JT | c | n'(JS)JT \rangle .
 \end{aligned}$$

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Analogous, for $L = L' = J \pm 1$ we find

$$\begin{aligned}
& \langle n(J \pm 1, 1)JT | \tilde{v} | n'(J \pm 1, 1)JT \rangle \\
& \stackrel{(2.11)}{=} \sum_{n''L''} \sum_{n'''L'''} \langle n''(L''S)JT | c | n(J \pm 1, 1)JT \rangle^* \langle n''(L''S)JT | v | n'''(L'''S)JT \rangle \\
& \quad \times \langle n'''(L'''S)JT | c | n'(J \pm 1, 1)JT \rangle \\
& \stackrel{(2.5)}{=} \sum_{n''} \sum_{n'''} \left(\langle n''(L \pm 1, 1)JT | c | n(J \pm 1, 1)JT \rangle^* \langle n''(J \pm 1, 1)JT | v | n'''(J \pm 1, 1)JT \rangle \right. \\
& \quad \times \langle n'''(J \pm 1, 1)JT | c | n'(J \pm 1, 1)JT \rangle + \langle n''(L \mp 1, 1)JT | c | n(J \pm 1, 1)JT \rangle^* \\
& \quad \times \langle n''(J \mp 1, 1)JT | v | n'''(J \pm 1, 1)JT \rangle \langle n'''(J \pm 1, 1)JT | c | n'(J \pm 1, 1)JT \rangle \\
& \quad + \langle n''(L \pm 1, 1)JT | c | n(J \pm 1, 1)JT \rangle^* \langle n''(J \pm 1, 1)JT | v | n'''(J \mp 1, 1)JT \rangle \\
& \quad \times \langle n'''(J \mp 1, 1)JT | c | n'(J \pm 1, 1)JT \rangle + \langle n''(L \mp 1, 1)JT | c | n(J \pm 1, 1)JT \rangle^* \\
& \quad \left. \times \langle n''(J \mp 1, 1)JT | v | n'''(J \mp 1, 1)JT \rangle \langle n'''(J \mp 1, 1)JT | c | n'(J \pm 1, 1)JT \rangle \right) . \tag{2.13}
\end{aligned}$$

And for $L = J \pm 1$ and $L' = J \mp 1$ we find

$$\begin{aligned}
& \langle n(J \pm 1, 1)JT | \tilde{v} | n'(J \mp 1, 1)JT \rangle \\
& \stackrel{(2.11)}{=} \sum_{n''L''} \sum_{n'''L'''} \langle n''(L''S)JT | c | n(J \pm 1, 1)JT \rangle^* \langle n''(L''S)JT | v | n'''(L'''S)JT \rangle \\
& \quad \times \langle n'''(L'''S)JT | c | n'(J \mp 1, 1)JT \rangle \\
& \stackrel{(2.5)}{=} \sum_{n''} \sum_{n'''} \left(\langle n''(L \pm 1, 1)JT | c | n(J \pm 1, 1)JT \rangle^* \langle n''(J \pm 1, 1)JT | v | n'''(J \pm 1, 1)JT \rangle \right. \\
& \quad \times \langle n'''(J \pm 1, 1)JT | c | n'(J \mp 1, 1)JT \rangle + \langle n''(L \mp 1, 1)JT | c | n(J \pm 1, 1)JT \rangle^* \\
& \quad \times \langle n''(J \mp 1, 1)JT | v | n'''(J \pm 1, 1)JT \rangle \langle n'''(J \pm 1, 1)JT | c | n'(J \mp 1, 1)JT \rangle \\
& \quad + \langle n''(L \pm 1, 1)JT | c | n(J \pm 1, 1)JT \rangle^* \langle n''(J \pm 1, 1)JT | v | n'''(J \mp 1, 1)JT \rangle \\
& \quad \times \langle n'''(J \mp 1, 1)JT | c | n'(J \mp 1, 1)JT \rangle + \langle n''(L \mp 1, 1)JT | c | n(J \pm 1, 1)JT \rangle^* \\
& \quad \left. \times \langle n''(J \mp 1, 1)JT | v | n'''(J \mp 1, 1)JT \rangle \langle n'''(J \mp 1, 1)JT | c | n'(J \mp 1, 1)JT \rangle \right) . \tag{2.14}
\end{aligned}$$

For $J = 0$, $S = 0$ and $T = 1$, the resulting matrix for $L = L' = 0$ is illustrated in figure 2.5 together with the corresponding uncorrelated interaction matrix. We observe that the correlation operator transformation truncates the large off-diagonal contributions and suppresses the matrix elements for small quantum numbers n and n' . Following from the unitarity verification of the previous section, the results are less reliable, the larger n and n' are.

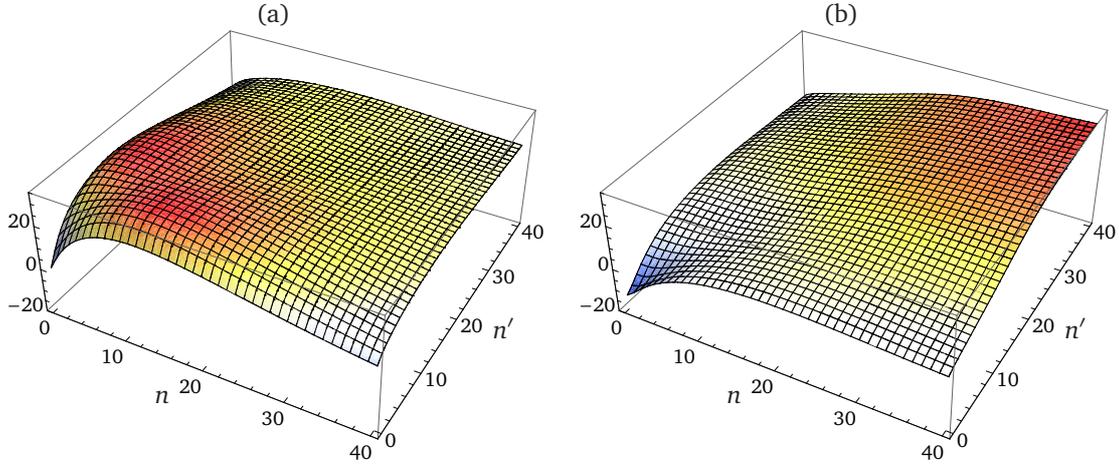


Figure 2.5: Uncorrelated (a) and correlated (b) interaction matrix elements for $J = 0$, $S = 0$, $T = 1$, $L = 0$ and $L' = 0$

2.2 Momentum Space Representation

In momentum space representation, the radial wave function ϕ is represented by the continuous relative momentum q . The relative wave functions are given by the radial momentum eigenfunctions

$$\langle r(LS)JT | q(LS)JT \rangle = \sqrt{\frac{2}{\pi}} j_L(qr), \quad (2.15)$$

which result from the partial wave decomposition of the plane waves [10]. The spherical Bessel functions

$$j_L(x) = (-1)^L x^L \left(\frac{1}{x} \frac{\partial}{\partial x} \right)^L \frac{\sin x}{x} \quad (2.16)$$

satisfy the closure relation

$$\int dr r^2 j_L(qr) j_L(q'r) = \frac{\pi}{2} \frac{\delta(q - q')}{qq'}. \quad (2.17)$$

2.2.1 Correlation Operator Matrix Elements

In analogy to the harmonic oscillator representation, we can derive the corresponding matrix elements of the correlation operator, this time using the formal framework of the momentum

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space representation:

$$\begin{aligned}
& \langle q(LS)JT | c_{\Omega} c_r | q'(L'S)JT \rangle \\
&= \sum_{L''S''J''T''} \int dr r^2 \langle q(LS)JT | c_{\Omega} | r(L''S'')J''T'' \rangle \langle r(L''S'')J''T'' | c_r | q'(L'S)JT \rangle \\
&= \sum_{L''S''J''T''} \int dr r^2 \mathcal{R}_-(r) \langle q(LS)JT | c_{\Omega} | r(L''S'')J''T'' \rangle \langle R_-(r)(L''S'')J''T'' | q'(L'S)JT \rangle \quad (2.18) \\
&\quad \times \delta_{L'L''} \delta_{SS''} \delta_{JJ''} \delta_{TT''} \\
&= \int dr r^2 \mathcal{R}_-(r) \langle q(LS)JT | c_{\Omega} | r(L'S)JT \rangle \langle R_-(r)(L'S)JT | q'(L'S)JT \rangle ,
\end{aligned}$$

where we have inserted the identity operator in position space representation, used equation (1.11) to evaluate the transformation of the central correlator and subsequently used the orthogonality of the radial momentum eigenfunctions. As for the matrix elements in harmonic oscillator representation, we distinguish three cases.

For $L = L' = J$ we find:

$$\begin{aligned}
& \langle q(JS)JT | c_{\Omega} c_r | q'(JS)JT \rangle \\
&\stackrel{(2.18)}{=} \int dr r^2 \mathcal{R}_-(r) \langle q(JS)JT | c_{\Omega} | r(JS)JT \rangle \langle R_-(r)(JS)JT | q'(JS)JT \rangle .
\end{aligned}$$

In accordance with equation (1.25), the tensor correlator does not have an effect here:

$$= \int dr r^2 \mathcal{R}_-(r) \langle q(JS)JT | r(JS)JT \rangle \langle R_-(r)(JS)JT | q'(JS)JT \rangle .$$

Analogous, for $L = L' = J \pm 1$ we get

$$\begin{aligned}
& \langle q(J \pm 1, 1)JT | c_{\Omega} c_r | q'(J \pm 1, 1)JT \rangle \\
&\stackrel{(2.18)}{=} \int dr r^2 \mathcal{R}_-(r) \langle q(J \pm 1, 1)JT | c_{\Omega} | r(J \pm 1, 1)JT \rangle \\
&\quad \times \langle R_-(r)(J \pm 1, 1)JT | q'(J \pm 1, 1)JT \rangle .
\end{aligned}$$

We use equation (1.26) to evaluate the transformation of the tensor correlator:

$$\begin{aligned}
 &= \int dr r^2 \mathcal{R}_-(r) \langle R_-(r)(J \pm 1, 1)JT | q'(J \pm 1, 1)JT \rangle \\
 &\quad \times \left(\langle q(J \pm 1, 1)JT | \cos \theta_J(r) | r(J \pm 1, 1)JT \rangle \right. \\
 &\quad \left. \pm \langle q(J \mp 1, 1)JT | \sin \theta_J(r) | r(J \pm 1, 1)JT \rangle \right) \\
 &= \int dr r^2 \mathcal{R}_-(r) \langle R_-(r)(J \pm 1, 1)JT | q'(J \pm 1, 1)JT \rangle \\
 &\quad \times \left(\cos \theta_J(r) \langle q(J \pm 1, 1)JT | r(J \pm 1, 1)JT \rangle \right. \\
 &\quad \left. \pm \sin \theta_J(r) \langle q(J \mp 1, 1)JT | r(J \pm 1, 1)JT \rangle \right) .
 \end{aligned}$$

The orthonormality of the radial momentum eigenfunctions leads to

$$\begin{aligned}
 &= \int dr r^2 \mathcal{R}_-(r) \langle R_-(r)(J \pm 1, 1)JT | q'(J \pm 1, 1)JT \rangle \\
 &\quad \times \cos \theta_J(r) \langle q(J \pm 1, 1)JT | r(J \pm 1, 1)JT \rangle .
 \end{aligned}$$

Finally, for $L = J \pm 1$ and $L' = J \mp 1$ we get

$$\begin{aligned}
 &\langle q(J \pm 1, 1)JT | c_\Omega c_r | q'(J \mp 1, 1)JT \rangle \\
 &\stackrel{(2.18)}{=} \int dr r^2 \mathcal{R}_-(r) \langle q(J \pm 1, 1)JT | c_\Omega | r(J \mp 1, 1)JT \rangle \\
 &\quad \times \langle R_-(r)(J \mp 1, 1)JT | q'(J \mp 1, 1)JT \rangle .
 \end{aligned}$$

Again we use equation (1.26) to evaluate the transformation of the tensor correlator:

$$\begin{aligned}
 &= \int dr r^2 \mathcal{R}_-(r) \langle R_-(r)(J \mp 1, 1)JT | q'(J \mp 1, 1)JT \rangle \\
 &\quad \times \left(\langle q(J \pm 1, 1)JT | \cos \theta_J(r) | r(J \mp 1, 1)JT \rangle \right. \\
 &\quad \left. \pm \langle q(J \mp 1, 1)JT | \sin \theta_J(r) | r(J \mp 1, 1)JT \rangle \right) \\
 &= \int dr r^2 \mathcal{R}_-(r) \langle R_-(r)(J \mp 1, 1)JT | q'(J \mp 1, 1)JT \rangle \\
 &\quad \times \left(\cos \theta_J(r) \langle q(J \pm 1, 1)JT | r(J \mp 1, 1)JT \rangle \right. \\
 &\quad \left. \pm \sin \theta_J(r) \langle q(J \mp 1, 1)JT | r(J \mp 1, 1)JT \rangle \right) .
 \end{aligned}$$

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As before, using the orthonormality of the radial momentum eigenfunctions we get

$$= \pm \int dr r^2 \mathcal{R}_-(r) \langle R_-(r)(J \mp 1, 1)JT | q'(J \mp 1, 1)JT \rangle \\ \times \sin \theta_J(r) \langle q(J \mp 1, 1)JT | r(J \mp 1, 1)JT \rangle .$$

For the sake of clarity, the resulting non-zero matrix elements $\langle q(JS)JT | c_\Omega c_r | q'(JS)JT \rangle$ for all combinations of L and L' are listed below.

$$\begin{aligned} \langle q(JS)JT | c_\Omega c_r | q'(JS)JT \rangle &= \int dr r^2 \mathcal{R}_-(r) \langle R_-(r)(JS)JT | q'(JS)JT \rangle \\ &\quad \times \langle r(JS)JT | q(JS)JT \rangle^* \\ \langle q(J \pm 1, 1)JT | c_\Omega c_r | q'(J \pm 1, 1)JT \rangle &= \int dr r^2 \mathcal{R}_-(r) \langle R_-(r)(J \pm 1, 1)JT | q'(J \pm 1, 1)JT \rangle \\ &\quad \times \cos \theta_J(r) \langle r(J \pm 1, 1)JT | q(J \pm 1, 1)JT \rangle^* \\ \langle q(J \pm 1, 1)JT | c_\Omega c_r | q'(J \mp 1, 1)JT \rangle &= \pm \int dr r^2 \mathcal{R}_-(r) \langle R_-(r)(J \mp 1, 1)JT | q'(J \mp 1, 1)JT \rangle \\ &\quad \times \sin \theta_J(r) \langle r(J \mp 1, 1)JT | q(J \mp 1, 1)JT \rangle^* . \end{aligned} \tag{2.19}$$

We observe that matrix elements with $L = L'$ in equation (2.19) cannot be evaluated numerically, because the integrand does not vanish for large values of r . For matrix elements with $L \neq L'$ the sine function suppresses the integrand, because $\lim_{r \rightarrow \infty} \theta_J(r) = 0$. In order to handle this problem, we reformulate the relevant matrix elements. Using the definitions

$$\begin{aligned} \tilde{j}_J(q'r) &= \sqrt{\frac{\pi}{2}} \mathcal{R}_-(r) \langle R_-(r)(J, 1)JT | q'(J, 1)JT \rangle , \\ \tilde{j}_{J \pm 1}(q'r) &= \sqrt{\frac{\pi}{2}} \cos \theta_J(r) \mathcal{R}_-(r) \langle R_-(r)(J \pm 1, 1)JT | q'(J \pm 1, 1)JT \rangle , \end{aligned} \tag{2.20}$$

the matrix elements read

$$\begin{aligned} \langle q(LS)JT | c_\Omega c_r | q'(LS)JT \rangle \\ = \frac{2}{\pi} \int dr r^2 j_L(qr) \tilde{j}_L(q'r) . \end{aligned}$$

Here, we first add and subtract $j_L(q'r)$, and subsequently separate the integral:

$$\begin{aligned} &= \frac{2}{\pi} \int dr r^2 j_L(qr) \left(\tilde{j}_L(q'r) - j_L(q'r) + j_L(q'r) \right) \\ &= \frac{2}{\pi} \int dr r^2 j_L(qr) \left(\tilde{j}_L(q'r) - j_L(q'r) \right) + \frac{2}{\pi} \int dr r^2 j_L(qr) j_L(q'r) . \end{aligned}$$

With the closure relation of the spherical Bessel functions (2.17) this reduces to

$$= \xi_L(q, q') + \frac{\delta(q - q')}{qq'} , \quad (2.21)$$

where we have introduced the definition

$$\xi_L(q, q') = \frac{2}{\pi} \int dr r^2 j_L(qr) \left(\tilde{j}_L(q'r) - j_L(q'r) \right) . \quad (2.22)$$

Since $\lim_{r \rightarrow \infty} R_-(r) = r$ and $\lim_{r \rightarrow \infty} \mathcal{R}_-(r) = 1$, we can infer from equation (2.20) that \tilde{j}_L and j_L are equal for large values of r . Consequently, the remaining integral $\xi_L(q, q')$ can be evaluated numerically.

For the same specific partial waves as in harmonic oscillator representation, the matrices corresponding to the matrix elements $\langle q(LS)JT | c_\Omega c_\tau | q'(L'S)JT \rangle - \frac{\delta(q-q')}{qq'} \delta_{LL'}$ for all possible combinations of L and L' are illustrated in figures 2.6 and 2.7. Again, we observe large off-diagonal contributions in all cases. We also note considerable fluctuations for the matrices with $L = L' = 0$ at very small momenta. Unlike in harmonic oscillator representation, a structural disparity of the matrices with $L \neq L'$ is evident. The matrix elements of the matrix corresponding to $L = J + 1$ and $L' = J - 1$ surpass the scale by one order of magnitude for very small momenta. Apart from that, all matrices are similar in structure.

2.2.2 Verification of Unitarity

In order to validate our numerical calculations and assess the applicability of our results, we employ the same approach as for the matrix elements in harmonic oscillator representation (see section 2.1.2). Accordingly, we have to verify that

$$\langle q(LS)JT | c^\dagger c | q'(L'S)JT \rangle \stackrel{!}{=} \langle q(LS)JT | q'(L'S)JT \rangle = \frac{\delta(q - q')}{qq'} \delta_{LL'} . \quad (2.23)$$

is satisfied. To this end, we express the matrix elements of $c^\dagger c$ in terms of the matrix elements listed above in (2.19) by inserting the identity operator in momentum space representation

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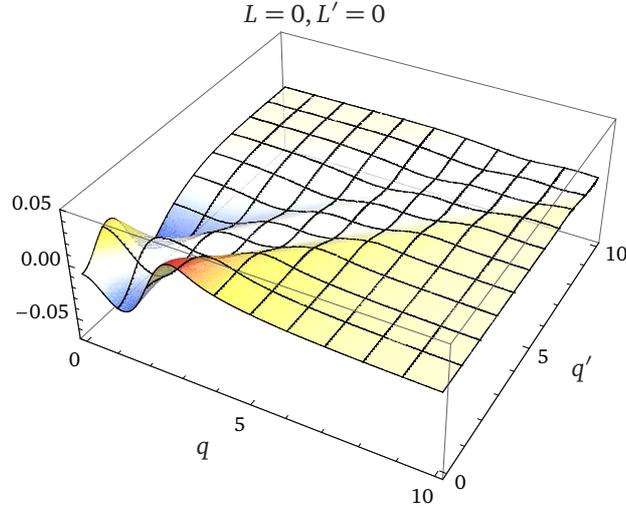


Figure 2.6: Correlation operator matrix elements for $J = 0$, $S = 0$ and $T = 1$ for the only possible combination of L and L'

and obtain

$$\begin{aligned}
 & \langle q(LS)JT | c^\dagger c | q'(L'S)JT \rangle \\
 &= \sum_{L''} \int dq'' q''^2 \langle q(LS)JT | c^\dagger | q''(L''S)JT \rangle \langle q''(L''S)JT | c | q'(L'S)JT \rangle \\
 &= \sum_{L''} \int dq'' q''^2 \langle q''(L''S)JT | c | q(LS)JT \rangle^* \langle q''(L''S)JT | c | q'(L'S)JT \rangle .
 \end{aligned} \tag{2.24}$$

Here, we differentiate between three cases. For $L = L' = J$ we find

$$\begin{aligned}
 & \langle q(JS)JT | c^\dagger c | q'(JS)JT \rangle \\
 & \stackrel{(2.24)}{=} \sum_{L''} \int dq'' q''^2 \langle q''(L''S)JT | c | q(JS)JT \rangle^* \langle q''(L''S)JT | c | q'(JS)JT \rangle \\
 & \stackrel{(2.19)}{=} \int dq'' q''^2 \langle q''(JS)JT | c | q(JS)JT \rangle^* \langle q''(JS)JT | c | q'(JS)JT \rangle .
 \end{aligned} \tag{2.25}$$

2.2 Momentum Space Representation

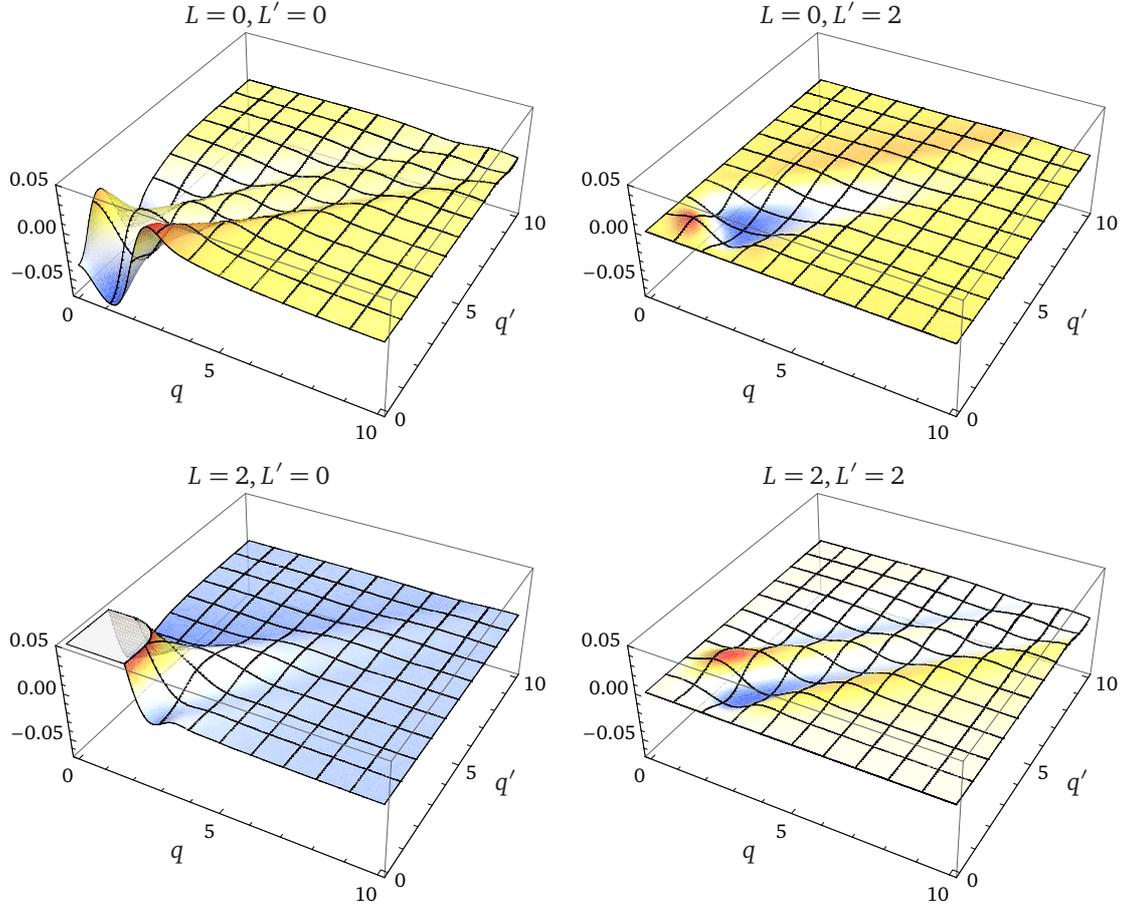


Figure 2.7: Correlation operator matrix elements for $J = 1$, $S = 1$ and $T = 0$ for all possible combinations of L and L'

Inserting equation (2.21) we get

$$\begin{aligned}
 &= \int dq'' q''^2 \left[\xi_J(q'', q) + \frac{\delta(q'' - q)}{q'' q} \right] \left[\xi_J(q'', q') + \frac{\delta(q'' - q')}{q'' q'} \right] \\
 &= \int dq'' q''^2 \left[\xi_J(q'', q) \xi_J(q'', q') + \frac{\delta(q'' - q)}{q'' q} \frac{\delta(q'' - q')}{q'' q'} \right. \\
 &\quad \left. + \xi_J(q'', q) \frac{\delta(q'' - q')}{q'' q'} + \xi_J(q'', q') \frac{\delta(q'' - q)}{q'' q} \right].
 \end{aligned}$$

Evaluating the integrals that include δ distributions yields

$$= \int dq'' q''^2 \xi_J(q'', q) \xi_J(q'', q') + \frac{\delta(q - q')}{qq'} + \xi_J(q', q) + \xi_J(q, q').$$

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Analogous, for $L = L' = J \pm 1$ we find

$$\begin{aligned}
& \langle q(J \pm 1, 1)JT | c^\dagger c | q'(J \pm 1, 1)JT \rangle \\
& \stackrel{(2.24)}{=} \sum_{L''} \int dq'' q''^2 \langle q''(L''S)JT | c | q(J \pm 1, 1)JT \rangle^* \langle q''(L''S)JT | c | q'(J \pm 1, 1)JT \rangle \\
& \stackrel{(2.19)}{=} \int dq'' q''^2 \left(\langle q''(J+1, 1)JT | c | q(J \pm 1, 1)JT \rangle^* \langle q''(J+1, 1)JT | c | q'(J \pm 1, 1)JT \rangle \right. \\
& \quad \left. + \langle q''(J-1, 1)JT | c | q(J \pm 1, 1)JT \rangle^* \langle q''(J-1, 1)JT | c | q'(J \pm 1, 1)JT \rangle \right) .
\end{aligned} \tag{2.26}$$

Inserting equation (2.21) we get

$$\begin{aligned}
& = \int dq'' q''^2 \left(\left[\xi_{J\pm 1}(q'', q) + \frac{\delta(q'' - q)}{q''q} \right] \left[\xi_{J\pm 1}(q'', q') + \frac{\delta(q'' - q')}{q''q'} \right] \right. \\
& \quad \left. + \langle q''(J \mp 1, 1)JT | c | q(J \pm 1, 1)JT \rangle^* \langle q''(J \mp 1, 1)JT | c | q'(J \pm 1, 1)JT \rangle \right) \\
& = \int dq'' q''^2 \xi_{J\pm 1}(q'', q) \xi_{J\pm 1}(q'', q') + \frac{\delta(q - q')}{qq'} + \xi_{J\pm 1}(q', q) + \xi_{J\pm 1}(q, q') \\
& \quad + \int dq'' q''^2 \langle q''(J \mp 1, 1)JT | c | q(J \pm 1, 1)JT \rangle^* \langle q''(J \mp 1, 1)JT | c | q'(J \pm 1, 1)JT \rangle .
\end{aligned}$$

Finally, for $L = J \pm 1$ and $L' = J \mp 1$ we find

$$\begin{aligned}
& \langle q(J \pm 1, 1)JT | c^\dagger c | q'(J \mp 1, 1)JT \rangle \\
& \stackrel{(2.24)}{=} \sum_{L''} \int dq'' q''^2 \langle q''(L''S)JT | c | q(J \pm 1, 1)JT \rangle^* \langle q''(L''S)JT | c | q'(J \mp 1, 1)JT \rangle \\
& \stackrel{(2.19)}{=} \int dq'' q''^2 \left(\langle q''(J+1, 1)JT | c | q(J \pm 1, 1)JT \rangle^* \langle q''(J+1, 1)JT | c | q'(J \mp 1, 1)JT \rangle \right. \\
& \quad \left. + \langle q''(J-1, 1)JT | c | q(J \pm 1, 1)JT \rangle^* \langle q''(J-1, 1)JT | c | q'(J \mp 1, 1)JT \rangle \right) .
\end{aligned} \tag{2.27}$$

Again, inserting equation (2.21) we get

$$\begin{aligned}
 &= \int dq'' q''^2 \left(\left[\xi_{J\pm 1}(q'', q) + \frac{\delta(q'' - q)}{q'' q} \right] \langle q''(J \pm 1, 1)JT | c | q'(J \mp 1, 1)JT \rangle \right. \\
 &\quad \left. + \langle q''(J \mp 1, 1)JT | c | q(J \pm 1, 1)JT \rangle \left[\xi_{J\mp 1}(q'', q') + \frac{\delta(q'' - q')}{q'' q'} \right] \right) \\
 &= \langle q(J \pm 1, 1)JT | c | q'(J \mp 1, 1)JT \rangle + \langle q'(J \mp 1, 1)JT | c | q(J \pm 1, 1)JT \rangle \\
 &\quad + \int dq'' q''^2 \xi_{J\pm 1}(q'', q) \langle q''(J \pm 1, 1)JT | c | q'(J \mp 1, 1)JT \rangle \\
 &\quad + \int dq'' q''^2 \xi_{J\mp 1}(q'', q') \langle q''(J \mp 1, 1)JT | c | q(J \pm 1, 1)JT \rangle .
 \end{aligned}$$

In order to evaluate the matrix elements $\langle q(LS)JT | c^\dagger c | q'(L'S)JT \rangle$ numerically, it is necessary to truncate the integration over q'' . Due to the large off-diagonal contributions of the correlation operator matrix mentioned before, the impact of truncation is more significant for large momenta q and q' . Analogous to our considerations in harmonic oscillator representation, we consequently expect unitarity to be satisfied well for small momenta q and q' only. For the same specific partial waves as in the previous section, the matrices corresponding to the matrix elements $\frac{\delta(q-q')}{qq'} \delta_{LL'} - \langle q(LS)JT | c^\dagger c | q'(L'S)JT \rangle$ are illustrated in figures 2.8 and 2.9 for all possible combinations of L and L' . Aside from so far unclear fluctuations at very small momenta q and q' , all matrices with $L = L'$ equal the zero matrix in good approximation for small momenta according to equation (2.23). However, the matrices with $L \neq L'$ have a fundamentally different structure. Contrary to our expectations, unitarity is satisfied well for large but not for very small momenta. In the region of very small momenta, the matrix elements surpass the scale by one order of magnitude. As of yet, the reason remains unclear.

2.2.3 Correlated Interaction Matrix Elements

As for the harmonic oscillator representation (see section 2.1.3), starting from the matrix elements of the uncorrelated interaction operator v , we can calculate the matrix elements of the correlated interaction operator \tilde{v} with the results of the previous sections. Equation

2 Correlated Interaction

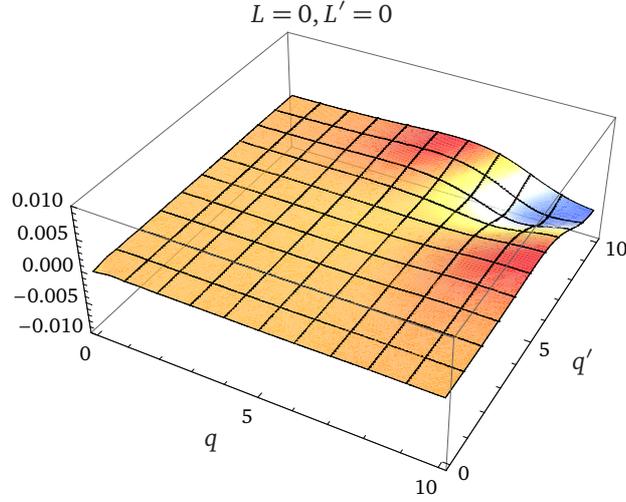


Figure 2.8: Unitarity verification for $J = 0$, $S = 0$ and $T = 1$ for the only possible combination of L and L'

(1.3) yields

$$\begin{aligned}
 & \langle q(LS)JT | \tilde{v} | q'(L'S)JT \rangle \\
 &= \langle q(LS)JT | c^\dagger v c | q'(L'S)JT \rangle \\
 &= \sum_{L''} \int dq'' q''^2 \sum_{L'''} \int dq''' q'''^2 \langle q(LS)JT | c^\dagger | q''(L''S)JT \rangle \langle q''(L''S)JT | v | q'''(L'''S)JT \rangle \\
 & \quad \times \langle q'''(L'''S)JT | c | q'(L'S)JT \rangle \\
 &= \sum_{L''} \int dq'' q''^2 \sum_{L'''} \int dq''' q'''^2 \langle q''(L''S)JT | c | q(LS)JT \rangle^* \langle q''(L''S)JT | v | q'''(L'''S)JT \rangle \\
 & \quad \times \langle q'''(L'''S)JT | c | q'(L'S)JT \rangle ,
 \end{aligned} \tag{2.28}$$

where we have inserted two identity operators in momentum space representation. We can evaluate this integral with equation (2.19). Again, we distinguish three cases. For $L = L' = J$

2.2 Momentum Space Representation

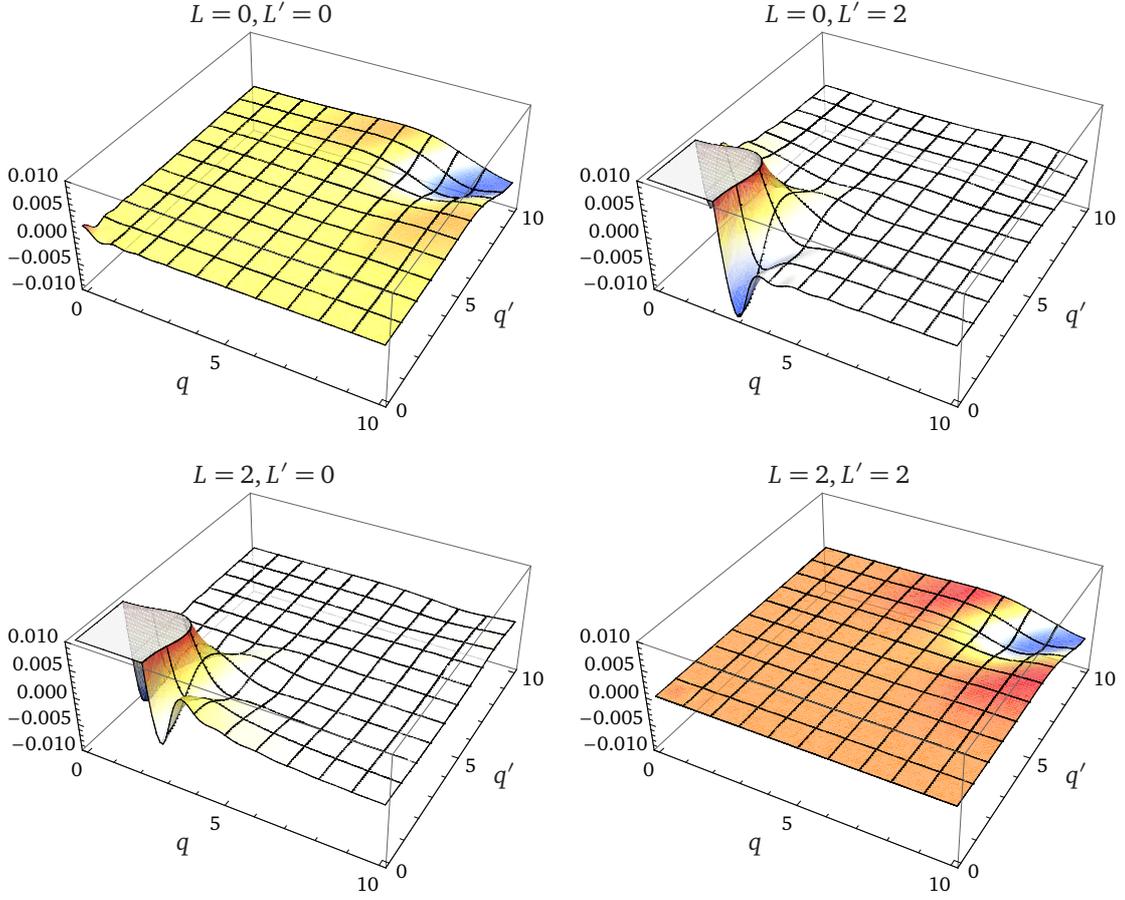


Figure 2.9: Unitarity verification for $J = 1$, $S = 1$ and $T = 0$ for all possible combinations of L and L'

we find

$$\begin{aligned}
 & \langle q(JS)JT | \tilde{v} | q'(JS)JT \rangle \\
 & \stackrel{(2.28)}{=} \sum_{L''} \int dq'' q''^2 \sum_{L'''} \int dq''' q'''^2 \langle q''(L''S)JT | c | q(JS)JT \rangle^* \\
 & \quad \times \langle q''(L''S)JT | v | q'''(L'''S)JT \rangle \langle q'''(L'''S)JT | c | q'(JS)JT \rangle \\
 & \stackrel{(2.19)}{=} \int dq'' q''^2 \int dq''' q'''^2 \langle q''(JS)JT | c | q(JS)JT \rangle^* \langle q''(JS)JT | v | q'''(JS)JT \rangle \\
 & \quad \times \langle q'''(JS)JT | c | q'(JS)JT \rangle .
 \end{aligned} \tag{2.29}$$

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In order to evaluate this numerically, we make us of equation (2.21) and get

$$\begin{aligned}
&= \int dq'' q''^2 \int dq''' q'''^2 \left[\xi_J(q'', q) + \frac{\delta(q'' - q)}{q'' q} \right] \langle q''(JS)JT | v | q'''(JS)JT \rangle \\
&\quad \times \left[\xi_J(q''', q') + \frac{\delta(q''' - q')}{q''' q'} \right] \\
&= \int dq'' q''^2 \int dq''' q'''^2 \left[\xi_J(q'', q) \xi_J(q''', q') + \frac{\delta(q'' - q)}{q'' q} \frac{\delta(q''' - q')}{q''' q'} \right. \\
&\quad \left. + \xi_J(q'', q) \frac{\delta(q''' - q')}{q''' q'} + \xi_J(q''', q') \frac{\delta(q'' - q)}{q'' q} \right] \langle q''(JS)JT | v | q'''(JS)JT \rangle \\
&= \int dq'' q''^2 \int dq''' q'''^2 \xi_J(q'', q) \xi_J(q''', q') \langle q''(JS)JT | v | q'''(JS)JT \rangle \\
&\quad + \langle q(JS)JT | v | q'(JS)JT \rangle \\
&\quad + \int dq'' q''^2 \xi_J(q'', q) \langle q''(JS)JT | v | q'(JS)JT \rangle \\
&\quad + \int dq''' q'''^2 \xi_J(q''', q') \langle q(JS)JT | v | q'''(JS)JT \rangle .
\end{aligned}$$

Analogous, for $L = L' = J \pm 1$ we find

$$\begin{aligned}
&\langle q(J \pm 1, 1)JT | \tilde{v} | q'(J \pm 1, 1)JT \rangle \\
&\stackrel{(2.28)}{=} \sum_{L''} \int dq'' q''^2 \sum_{L'''} \int dq''' q'''^2 \langle q''(L''S)JT | c | q(J \pm 1, 1)JT \rangle^* \\
&\quad \times \langle q''(L''S)JT | v | q'''(L'''S)JT \rangle \langle q'''(L'''S)JT | c | q'(J \pm 1, 1)JT \rangle \\
&\stackrel{(2.19)}{=} \int dq'' q''^2 \int dq''' q'''^2 \left(\langle q''(J \pm 1, 1)JT | c | q(J \pm 1, 1)JT \rangle^* \right. \\
&\quad \times \langle q''(J \pm 1, 1)JT | v | q'''(J \pm 1, 1)JT \rangle \langle q'''(J \pm 1, 1)JT | c | q'(J \pm 1, 1)JT \rangle \\
&\quad + \langle q''(J \mp 1, 1)JT | c | q(J \pm 1, 1)JT \rangle^* \langle q''(J \mp 1, 1)JT | v | q'''(J \pm 1, 1)JT \rangle \\
&\quad \times \langle q'''(J \pm 1, 1)JT | c | q'(J \pm 1, 1)JT \rangle + \langle q''(J \pm 1, 1)JT | c | q(J \pm 1, 1)JT \rangle^* \\
&\quad \times \langle q''(J \pm 1, 1)JT | v | q'''(J \mp 1, 1)JT \rangle \langle q'''(J \mp 1, 1)JT | c | q'(J \pm 1, 1)JT \rangle \\
&\quad \left. + \langle q''(J \mp 1, 1)JT | c | q(J \pm 1, 1)JT \rangle^* \langle q''(J \mp 1, 1)JT | v | q'''(J \mp 1, 1)JT \rangle \right. \\
&\quad \left. \times \langle q'''(J \mp 1, 1)JT | c | q'(J \pm 1, 1)JT \rangle \right) . \tag{2.30}
\end{aligned}$$

2.2 Momentum Space Representation

As before, we have to use equation (2.21) for numerical evaluation. For simplicity, we omit a detailed derivation here. Finally, for $L = J \pm 1$ and $L' = J \mp 1$ we find

$$\begin{aligned}
& \langle q(J \pm 1, 1)JT | \tilde{v} | q'(J \mp 1, 1)JT \rangle \\
& \stackrel{(2.28)}{=} \sum_{L''} \int dq'' q''^2 \sum_{L'''} \int dq''' q'''^2 \langle q''(L''S)JT | c | q(J \pm 1, 1)JT \rangle^* \\
& \quad \times \langle q''(L''S)JT | v | q'''(L'''S)JT \rangle \langle q'''(L'''S)JT | c | q'(J \mp 1, 1)JT \rangle \\
& \stackrel{(2.19)}{=} \int dq'' q''^2 \int dq''' q'''^2 \left(\langle q''(J \pm 1, 1)JT | c | q(J \pm 1, 1)JT \rangle^* \right. \\
& \quad \times \langle q''(J \pm 1, 1)JT | v | q'''(J \pm 1, 1)JT \rangle \langle q'''(J \pm 1, 1)JT | c | q'(J \mp 1, 1)JT \rangle \\
& \quad + \langle q''(J \mp 1, 1)JT | c | q(J \pm 1, 1)JT \rangle^* \langle q''(J \mp 1, 1)JT | v | q'''(J \pm 1, 1)JT \rangle \\
& \quad \times \langle q'''(J \pm 1, 1)JT | c | q'(J \mp 1, 1)JT \rangle + \langle q''(J \pm 1, 1)JT | c | q(J \pm 1, 1)JT \rangle^* \\
& \quad \times \langle q''(J \pm 1, 1)JT | v | q'''(J \mp 1, 1)JT \rangle \langle q'''(J \mp 1, 1)JT | c | q'(J \mp 1, 1)JT \rangle \\
& \quad + \langle q''(J \mp 1, 1)JT | c | q(J \pm 1, 1)JT \rangle^* \langle q''(J \mp 1, 1)JT | v | q'''(J \mp 1, 1)JT \rangle \\
& \quad \left. \times \langle q'''(J \mp 1, 1)JT | c | q'(J \mp 1, 1)JT \rangle \right) . \tag{2.31}
\end{aligned}$$

Again, equation (2.21) is required for numerical evaluation. As before, we omit a detailed derivation for the sake of simplicity.

In principle, we can now calculate the resulting matrices numerically. However, the unexpected results of the unitarity verification imply that such results cannot be considered reliable, which is why we do not present them here.

2 *Correlated Interaction*

CHAPTER 3

SUMMARY AND OUTLOOK

As described in the introduction, the interaction between nucleons can be deduced by considering both general symmetry requirements and empirical findings. With a nucleon-nucleon interaction available, there are different ways of solving the nuclear many-body problem. While *ab initio* methods are not practicable for nuclei with large mass numbers due to the computational costs, mean field methods are unable to account for the correlations induced by realistic nucleon-nucleon interactions.

In chapter 1 we presented the Unitary Correlation Operator Method, a concept that circumvents these limitations by imprinting the dominant short-range central and tensor correlations into a many-body state via the transformation of the correlation operator. In chapter 2, we derived the matrix elements of the correlation operator in both harmonic oscillator and momentum space representation. We also examined a method to assess the applicability of our findings, which revealed that the results in momentum space representation are not reliable yet. Further research is required to discover the reason and solution of this problem. On the basis of our studies of the correlation operator, we subsequently developed a formalism with which we can calculate matrix elements of an arbitrary potential that take the central and the tensor correlations into account in both representations.

Since many modern nucleon-nucleon interactions are only formulated via their matrix elements in these representations, this formalism can be used to solve the nuclear many-body problem based upon these interactions.

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DECLARATION OF AUTHENTICITY

I hereby declare that this thesis is my own original work and that all sources have been accurately reported and acknowledged.

Christoph Popa, July 2008