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Orthonormalization procedure for chiral effective nuclear field theory[#1]

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Abstract

We show that the $\hat{Q}$-box expansion of nuclear many-body physics can be applied in nuclear effective field theory with explicit pions and external sources. We establish the corresponding power counting and give an algorithm for the construction of a hermitean and energy-independent potential for arbitrary scattering processes on nucleons and nuclei to a given order in the chiral expansion. Various examples are discussed in some detail.

Keywords: chiral effective field theory theory, few-nucleon processes

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1 Introduction and summary

Effective field theory methods applied to few-nucleon systems have become a powerful tool to establish a systematic and precise formulation of nuclear physics consistent with the symmetries of QCD, in particular its spontaneously and explicitly broken chiral symmetry. The field was initiated by a series of papers of Weinberg [1, 2, 3] and has matured considerably. Recently, two-nucleon dynamics based on effective field theory (EFT) with explicit pions [#2] has been worked out at next-to-next-to-next-to-leading order (NNNLO), see [4, 5] [#3]. Due to the appearance of shallow bound states a purely perturbative treatment like in chiral perturbation theory for systems with pions or with one nucleon is inappropriate. However, as stressed already by Weinberg, one can apply the power counting in the construction of the so-called effective potential. Through iteration of this effective potential one obtains the full physical scattering amplitude. In the case of nucleon-nucleon scattering, it was shown in [1] that the power counting is violated if one considers diagrams containing two-nucleon intermediate states. From that, the simplest definition of the effective potential can be given as follows: the effective potential is the sum of all time-ordered diagrams which contain in each intermediate state at least one pion. No violation of the power counting appears on the level of the effective potential, thus it can be constructed perturbatively in terms of the usual small parameters q/Λ_χ and M_π/Λ_χ, with q a generic external momentum, M_π the pion mass and $\Lambda_\chi \simeq 1\,\text{GeV}$ the scale of chiral symmetry breaking. The extension of these arguments to pion production or the inclusion of the $\Delta(1232)$ is straightforward if one takes into account the new scales appearing in these cases (see e.g. [6]). We will not consider such extensions here specifically, although our formalism is general enough to include these. Once the effective potential is constructed to a given order in the chiral expansion, the full T-matrix generating the bound and scattering states can be calculated by solving the Lippmann-Schwinger equation, $T = V_{\text{eff}} + V_{\text{eff}} G_0 T$, with G_0 the two-nucleon propagator. Even though this definition of the effective potential is very simple, one encounters some disadvantages. The potential is energy-dependent and not hermitean. This makes it difficult to apply it to scattering processes involving more than two nucleons. A solution to this problem was given by Epelbaum and collaborators [7], who showed that the method of unitary transformations developed by Fukuda, Sawada and Taketani [8] and by Okubo [9] can be applied to generate an energy-independent and hermitean potential consistent with the power counting of chiral perturbation theory (the effective potential). While this method is quite powerful, it suffers from the disadvantage that for different processes one has to define different model spaces and each time to construct the operator A, which parameterizes the corresponding unitary transformation, and to deduce the resulting hermitean effective Hamiltonian. We propose here another scheme based on the $\hat{Q}$-box expansion of Kuo and collaborators [10, 11]. The main results of this study are:

i) We have shown that the $\hat{Q}$-box expansion respects the chiral expansion: only a finite number of $\hat{Q}$-boxes contribute to the effective potential at a given chiral order.

ii) We have constructed an explicit algorithm that allows one to construct the effective potential for any process involving nucleons, pions and photons (or other external sources) to a given order in the chiral expansion, see section 5.

iii) We have shown for various examples that when one requires the on-shell condition to the asymptotic states, one recovers the expressions based on time-ordered perturbation theory, as it should be.

iv) An explicit application of the method developed here is the calculation of the fourth-order corrections to the three-body contributions in neutral pion electroproduction off the deuteron, see [12].

The manuscript is organized as follows. In section 2 we briefly review Weinberg's approach to the chiral dynamics of few-nucleon systems and the corresponding power counting. A general derivation of the hermitean effective potential is given in sec. 3, following closely [13]. The $\hat{Q}$-box expansion is discussed in sec. 4. These three sections do not contain new results but are needed to keep our presentation self-contained. Sec. 5 contains our central results. We show that the $\hat{Q}$-box expansion is consistent with the chiral expansion and further give an explicit algorithm to construct the hermitean effective potential to a given chiral order. Some leading order considerations are discussed in sec. 6, in particular the role of the so-called Okubo corrections (wave function orthonormalization diagrams). Various technicalities are relegated to the appendices.

[#2] We do not consider the so-called pionless EFT in what follows.

[#3] Note that only in [5] a detailed analysis of the theoretical uncertainties at this order is given as it is required for any sensible EFT analysis.

2 A brief review of Weinberg's approach to chiral few-nucleon dynamics

This section contains a very brief introduction to chiral perturbation theory with two (or more) nucleons and serves mainly to fix the notation. As pointed out by Weinberg [1, 2, 3] some years ago, for processes involving two or more nucleons the standard power counting of chiral perturbation theory is valid only for a subset of diagrams. This subset consists of the time-ordered diagrams which in every intermediate state contain at least one pion (or delta). The sum of all the diagrams from this subset is called the effective potential, denoted by $V_{\rm eff}^{NN}$. The whole transition matrix or nuclear wave function can be computed numerically in the standard way by solving the inhomogeneous or homogeneous Lippmann-Schwinger equation with the given effective potential. For a more detailed description, see e.g. [14]

If we are interested in pion scattering processes on nucleons or nuclei, we can obviously proceed in a similar way and define an effective potential composed of diagrams, which contain in every intermediate state at least two pions (or deltas). In this way we get an effective potential matrix

$$V_{\rm eff} = \begin{pmatrix} \langle \pi NN|V_{\rm eff}|\pi NN\rangle & \langle \pi NN|V_{\rm eff}|NN\rangle \\ \langle NN|V_{\rm eff}|\pi NN\rangle & \langle NN|V_{\rm eff}|NN\rangle \end{pmatrix}, \tag{1}$$

where NN denote here a state with two or more than two nucleons. The elastic pion scattering potential can be decomposed in two parts as has been shown in Fig. 1: the first part contains all diagrams from the effective potential with the pion acting as a spectator. Let us denote it by $\langle \pi NN|V_{\rm eff}^{S}|\pi NN\rangle$. The second part contains all other possible diagrams. It is obvious that the first part is given by the usual effective potential $V_{\rm eff}^{NN}$ multiplied by the three dimensional delta function of the pion spectator. If we want to describe scattering processes on nuclei, it is useful to define the well–known Lovelace operator [15], called here the irreducible kernel K:

$$K = V_{\rm eff}^{i} + V_{\rm eff}^{f} \frac{1}{E - H_0 - V_{\rm eff} + i\epsilon} V_{\rm eff}^{i}, \tag{2}$$

where E denotes the total energy of the system and the potentials $V_{\rm eff}^{i}$ and $V_{\rm eff}^{f}$ are given by

$$V_{\rm eff}^{i} = H_0 + V_{\rm eff} - H_0^{i}, \quad V_{\rm eff}^{f} = H_0 + V_{\rm eff} - H_0^{f}, \tag{3}$$

and H_0, H_0^{i} and H_0^{f} denote the free Hamilton operators of the particles in the intermediate state, of the initial and of the final asymptotic states, respectively. In the case of pion scattering, e.g., $V_{\rm eff}^{i}$ and $V_{\rm eff}^{f}$ are given by the effective potential without the pion spectator contribution:

$$V_{\rm eff}^{i} = V_{\rm eff}^{f} = V_{\rm eff} - \begin{pmatrix} \langle \pi NN|V_{\rm eff}^{S}|\pi NN\rangle & 0 \\ 0 & 0 \end{pmatrix}. \tag{4}$$

All diagrams from K are called irreducible and all others are called reducible. To calculate the transition amplitude for scattering processes on nuclei, one has to convolute the irreducible kernel K with the corresponding nuclear wave functions. Since in every intermediate state of the kernel K the chiral counting can be applied (no infrared singularities appear if the nucleon mass approaches infinity), one can calculate it perturbatively. The simultaneous expansion both in small momenta (masses) of Goldstone-bosons and in one over the nucleon mass can be performed. The $1/m$ Taylor series expansion within the potentials can be done, since no unitarity cuts can appear there (note that we always define the model space such that the potentials are real). The cuts, which are responsible for the imaginary part of the scattering amplitude, are all outside the potentials (the inside/outside refers to the structure of the kernel given in Eq. (2)), where the trivial $1/m$ Taylor expansion does not make sense. However outside the potentials one can perform the $1/m$ expansion within the energy denominator, which is symbolically given in the following equation:

$$\frac{1}{E - E' + i\epsilon} = \frac{1}{(E - E')_0 + A/m + B/m^2 + \cdots + i\epsilon}. \tag{5}$$

Here $(E - E')_0$ denotes the corresponding energy difference $E - E'$ in the static limit. In some cases the nucleon recoil corrections, denoted here by A/m, are sizeable and can not be neglected, for more detailed discussion

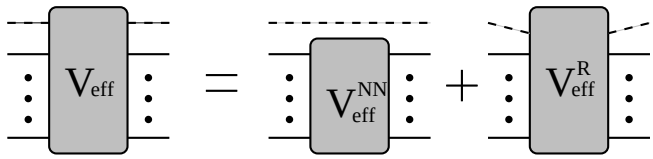

Figure 1: A nuclear potential decomposed into the pion spectator and the interaction part.

of this topic see e.g. [16]. The power counting for a given diagram from the irreducible kernel K or nuclear potential is given by [3]

$$\nu = 4 - N - 2C + 2L + \sum_i V_i \Delta_i, \quad \Delta_i = d_i + \frac{1}{2} n_i - 2, \tag{6}$$

where N, C, L, V_i, d_i and n_i are the number of nucleons, of connected pieces, of loops, of vertices of type i, of derivatives (or powers of the pion mass) at the vertex i and of nucleons at the vertex i, respectively. In order to calculate a scattering process up to a given chiral order ν_{max} we have to sum up all the diagrams with $\nu \leq \nu_{max}$ from the kernel K and convolute them with the chiral nuclear wave functions fixed by the corresponding nuclear potential calculated up to order $\nu_{max} + 3$. The added 3 here guarantees that the operators V^S_{eff} and K are of the same chiral order [#4].

Although all that looks nice, one well known disadvantage appears: the effective potentials defined in this simple way are energy-dependent and non-hermitean. This makes it difficult to apply the formalism to the processes, where more than two nucleons are involved. Epelbaoum et al. [7] suggested another construction of effective potential using the techniques of unitary transformation, firstly introduced by Okubo [9] many years ago. They showed explicitly, how to construct the hermitean energy-independent N-nucleon potential up to a given order in chiral perturbation theory. To be consistent with this picture we have to extend the given construction to the scattering processes on nucleons and nuclei. The main purpose of this manuscript is to give such an extension, such that both the nuclear wave functions on the one hand and the irreducible kernel on the other hand were constructed using hermitean energy-independent potentials in a unified way.

3 Hermitean effective potential

To derive the general effective potential, we proceed in the manner of Suzuki and Okamoto [13]. For earlier and related work, see e.g. [17, 18, 19, 20, 21, 22, 23]. Let the full Fock-space $\mathcal{H}$ of all physical states be described as a direct sum of a model subspace $\mathcal{H}_{\mathcal{M}}$ and its complementary space $\mathcal{H}_{\mathcal{R}}$,

$$\mathcal{H} \quad = \quad \mathcal{H}_{\mathcal{M}} \oplus \mathcal{H}_{\mathcal{R}}. \tag{7}$$

Let P and Q be projection operators onto these two subspaces,

$$P, Q : \mathcal{H} \quad \rightarrow \quad \mathcal{H} \tag{8}$$

such that $Im[P] \subset \mathcal{H}_{\mathcal{M}}$, $Im[Q] \subset \mathcal{H}_{\mathcal{R}}$, $PQ = QP = 0$ and $P + Q = 1$, with $1 = Id$ the Identity operator $Id : \mathcal{H} \rightarrow \mathcal{H}$. Let $A : \mathcal{H} \rightarrow \mathcal{H}$ be an operator with the following property, $A[\mathcal{H}_{\mathcal{M}}] \subset \mathcal{H}_{\mathcal{R}}$ and $A\,[\mathcal{H}_{\mathcal{R}}] = 0$, such that it maps the states from the model space $\mathcal{H}_{\mathcal{M}}$ to the states from the complementary space $\mathcal{H}_{\mathcal{R}}$. From this property it follows immediately

$$A \quad = \quad QAP\ , \tag{9}$$

$$AQ \quad = \quad 0\ , \tag{10}$$

$$PA \quad = \quad 0\ , \tag{11}$$

and

$$A^2 \quad = \quad 0\ . \tag{12}$$

[#4] Note that V^S_{eff} is given by a nuclear potential multiplied by the pion spectator delta function, which decreases the chiral dimension by -3.

Now we define an operator $X(n)$ by

$$X(n) \;=\; (1+A)(1+A^\dagger A+AA^\dagger)^n, \tag{13}$$

with n a real number. The inverse of $X(n)$ is

$$X^{-1}(n) \;=\; (1+A^\dagger A+AA^\dagger)^{-n}(1-A). \tag{14}$$

The above relation can be verified by using the fact that $(1-A)(1+A)=1$. The stationary Schrödinger equation of the original problem $H\Psi=E\Psi$, where $H=H_0+V$ is the Hamiltonian of the physical problem represented as a sum of the free and interacting parts H_0 and V, can be transformed to

$$X^{-1}(n)HX(n)X^{-1}(n)\Psi \;=\; EX^{-1}(n)\Psi. \tag{15}$$

Suppose that the transformed operator $X^{-1}(n)HX(n)$ fulfills for $n=0$ the decoupling equation

$$QX^{-1}(0)HX(0)P \;=\; Q(H+[H,A]-AHA)P \;=\; 0. \tag{16}$$

This is exactly the equation of Okubo [9] for the operator A. The above equation leads to the general decoupling equation

$$QX^{-1}(n)HX(n)P \;=\; (Q+AA^\dagger)^{-n}QX^{-1}(0)HX(0)P(P+A^\dagger A)^n \;=\; 0, \tag{17}$$

where we have used the fact, that

$$(1+A^\dagger A+AA^\dagger)^nP \;=\; (P+A^\dagger A)^n, \tag{18}$$

$$Q(1+A^\dagger A+AA^\dagger)^n \;=\; (Q+AA^\dagger)^n. \tag{19}$$

If we now start from the effective equation in the model space

$$PX^{-1}(n)HX(n)P\Phi \;=\; E\Phi, \quad \Phi\in\mathcal{H}_{\mathcal{M}} \tag{20}$$

we get (because of the decoupling equation)

$$X^{-1}(n)HX(n)\Phi \;=\; E\Phi. \tag{21}$$

Multiplying this equation by $X(n)$ from the left brings us to the original Schrödinger equation:

$$H\Psi \;=\; E\Psi, \tag{22}$$

with $\Psi=X(n)\Phi$. Let us introduce at this stage some important notation for the effective Hamiltonian and the potential:

$$H_{\rm eff}(n) \;:=\; PX^{-1}(n)HX(n)P \;=\; PH_0P+V_{\rm eff}(n) \tag{23}$$

To study the properties of $V_{\rm eff}(n)$, we multiply the Eq. (16) from the left by $A^\dagger$ and conjugate the last equation:

$$PA^\dagger QHP+PA^\dagger QHQAP-PA^\dagger APHP-PA^\dagger APHQAP \;=\; 0, \tag{24}$$

$$PHQAP+PA^\dagger QHQAP-PHPA^\dagger AP-PA^\dagger QHPA^\dagger AP \;=\; 0. \tag{25}$$

Eliminating the QHQ-term from the above equations we get

$$P(1+A^\dagger)HP(P+A^\dagger A) \;=\; (P+A^\dagger A)PH(1+A)P. \tag{26}$$

The effective Hamiltonian and its adjoint have the form

$$\begin{aligned} H_{\rm eff}(n) &= (P+A^\dagger A)^{-n}(1-A)H(1+A)(P+A^\dagger A)^n \\ &= (P+A^\dagger A)^{-n}PH(1+A)P(P+A^\dagger A)^n, \end{aligned} \tag{27}$$

$$\begin{aligned} H^\dagger_{\rm eff}(n) &= (P+A^\dagger A)^n(1+A^\dagger)H(1-A^\dagger)(P+A^\dagger A)^{-n} \\ &= (P+A^\dagger A)^nP(1+A^\dagger)HP(P+A^\dagger A)(P+A^\dagger A)^{-n-1} \\ &= (P+A^\dagger A)^{n+1}PH(1+A)(P+A^\dagger A)^{-n-1}. \end{aligned} \tag{28}$$

So we obtain the relation

$$H_{\rm eff}(n) \;=\; H^{\dagger}_{\rm eff}(-n-1). \tag{29}$$

From the above relation we see that $H_{\rm eff}(n)$ becomes hermitean when $n=-1/2$.

For practical purposes two effective interactions are of special importance. The first one is $H_{\rm eff}(0)$, which has a relatively simple form

$$H_{\rm eff}(0) \;=\; PHP + PHQA \;=\; PH_0P + R, \tag{30}$$

with the non-hermitean potential, denoted by

$$R = V_{\rm eff}(0) \;=\; PVP + PVQA. \tag{31}$$

Because of its simplicity this energy-independent non-hermitean potential has rich applications in nuclear physics.

Another important effective Hamiltonian is $H_{\rm eff}(-1/2)$, which is hermitean. Its explicit form is

$$H_{\rm eff}(-1/2) \;=\; (P+A^{\dagger}A)^{1/2}H(P+A)(P+A^{\dagger}A)^{-1/2} \;=\; PH_0P + W, \tag{32}$$

with the hermitean potential, denoted by $W = V_{\rm eff}(-1/2)$. The hermitean theory is more complicated than the standard non-hermitean theory, but has an advantage that the wave functions, which come from the solution of the effective Schrödinger equation, are orthonormal. To see this, let us define an operator

$$G = \operatorname{arctanh}\left(A - A^{\dagger}\right). \tag{33}$$

It can be shown that the following relation is valid [20]:

$$\exp(G) = \left(1 + A - A^{\dagger}\right)\left(1 + A^{\dagger}A + AA^{\dagger}\right)^{-1/2}. \tag{34}$$

Using Eq. (18) we immediately see that

$$\exp(G)P = (1+A)\left(P + A^{\dagger}A\right)^{-1/2} = X(-1/2)P. \tag{35}$$

Let $\{|\psi_n\rangle\}$ denote a set of orthonormal eigenstates of the Hamiltonian H. The corresponding eigenstates $\{|\phi_n\rangle\}$ of effective Hamiltonian are related to the original one by

$$|\psi_n\rangle = X(-1/2)|\phi_n\rangle = X(-1/2)P|\phi_n\rangle = \exp(G)P|\phi_n\rangle, \tag{36}$$

such that we get for the effective eigenstates

$$|\phi_n\rangle = \exp(-G)|\psi_n\rangle. \tag{37}$$

The orthonormality of the effective eigenstates follows now directly from the unitarity of $\exp(G)$:

$$\langle\phi_n|\phi_m\rangle = \langle\psi_n|\exp(G)\exp(-G)|\psi_m\rangle = \langle\psi_n|\psi_m\rangle = \delta_{n,m}. \tag{38}$$

Now let us discuss some interesting relations between hermitean and non-hermitean potentials. One can show the following general relation [19]

$$W \;=\; PVP + \sum_{m,n=0}^{\infty} F(m,n)\left((A^{\dagger}A)^m PVQA(A^{\dagger}A)^n + h.c.\right), \tag{39}$$

with the function $F(m,n)$ defined as coefficients of the Taylor series of

$$f(x,y) \;=\; \frac{\sqrt{1+x}}{\sqrt{1+x}+\sqrt{1+y}} \;=\; \sum_{m,n=0}^{\infty} F(m,n)x^m y^n. \tag{40}$$

Table 1: The values of $F(m,n)$.

(m,n)	$(0,0)$	$(0,1)$	$(1,0)$	$(0,2)$	$(1,1)$	$(2,0)$
$F(m,n)$	$1/2$	$-1/8$	$1/8$	$1/16$	0	$-1/16$

From the property $f(x,y)+f(y,x)=1$ we have the anti-symmetry relation

$$F(m,n) \quad = \quad -F(n,m), \tag{41}$$

unless $m=n=0$. The values of $F(m,n)$ for small m and n are given in Table 1. Due to the anti-symmetry relation (41) and from the definition of R in Eq. (31), we can write W in another form as

$$W \quad = \quad \frac{R+R^\dagger}{2} + \sum_{m+n>0} F(m,n)(A^\dagger A)^m (R-R^\dagger)(A^\dagger A)^n, \tag{42}$$

where the summation runs over zero or all positive integers except $m=n=0$. The expression of W in the above equation clarifies how the non-hermiticity term $\sim (R-R^\dagger)$ contributes to the hermitean effective interaction W. The first two terms in the expansion of W are given by

$$W \quad = \quad \frac{1}{2}(R+R^\dagger) + \frac{1}{8}\left((A^\dagger A)(R-R^\dagger)+h.c.\right) - \frac{1}{16}\left((A^\dagger A)^2(R-R^\dagger)+h.c.\right) + \dots \ . \tag{43}$$

This formula will be useful for our later investigations.

4 The $\hat{Q}$-box expansion of the effective interaction

We are now interested in the solution of the decoupling equation (16) for the operator A. Once we have constructed the operator A we are able to give an explicit form for the effective potentials R and W. For this reason we define a so called $\hat{Q}$-box, which was first introduced by Kuo and collaborators[10] in the study of the folded diagram expansion of an effective potential:

$$\hat{Q}(E) \quad = \quad PVP + PVQ\frac{1}{E-QHQ}QVP. \tag{44}$$

The physical meaning of this object is very familiar. It is nothing else but the sum of all time-ordered diagrams, which do not contain any model-space intermediate states. For example if one fixes the model-space as a space of all pure nucleon states, then every diagram from the $\hat{Q}$-box has to contain at least one pion or delta in every intermediate state. Some lowest order diagrams of a $\hat{Q}$-box in the case of nucleon-nucleon scattering are given in Figure 2. We also want to introduce higher $\hat{Q}$-boxes as

$$\hat{Q}_n(E_1,...,E_{n+1}) \quad = \quad (-1)^n PVQ\frac{1}{(E_1-QHQ)\cdots(E_{n+1}-QHQ)}QVP. \tag{45}$$

Higher $\hat{Q}$-boxes can be easily derived from the original $\hat{Q}$-box through the relation [22]

$$\hat{Q}_n(E_1,...,E_{n+1}) \quad = \quad \sum_{k=1}^{n+1} C_k(E_1,...,E_{n+1})\hat{Q}(E_k) \tag{46}$$

where

$$C_k(E_1,...,E_{n+1}) \quad = \quad \frac{1}{(E_k-E_1)\cdots(E_k-E_{k-1})(E_k-E_{k+1})\cdots(E_k-E_{n+1})}. \tag{47}$$

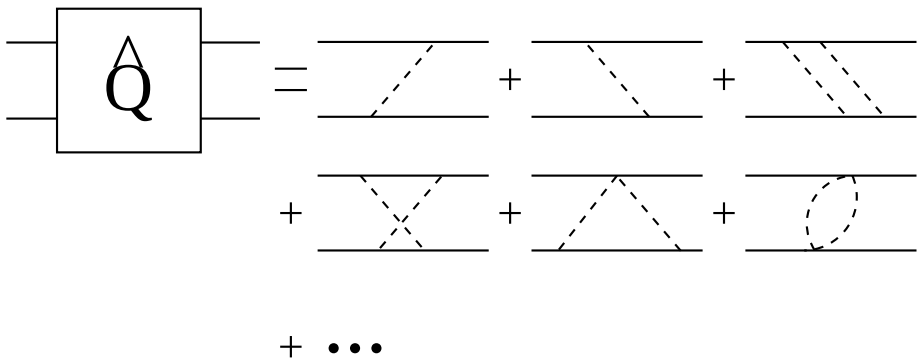

Figure 2: Some lowest order diagrams of a $\hat{Q}$-box in the case of nucleon-nucleon scattering.

If at least two of the energies mentioned above are equal, one has to understand Eq. (46) as a limit. To make this clear, let us look for example at $\hat{Q}_1(E_1, E_2)$-box, with the energies $E_1 = E_2$:

$$\begin{aligned}
& \lim_{E_1\to E_2} \left(\frac{1}{(E_1-E_2)}\hat{Q}\left(E_1\right) + \frac{1}{(E_2-E_1)}\hat{Q}\left(E_2\right)\right) \\
= & \lim_{E_1\to E_2} \left(\frac{1}{(E_1-E_2)}PVP + \frac{1}{(E_2-E_1)}PVP\right) \\
+ & \lim_{E_1\to E_2} PVQ\frac{1}{E_1-E_2}\left(\frac{1}{E_1-QHQ} - \frac{1}{E_2-QHQ}\right)QVP \\
= & \lim_{E_1\to E_2} PVQ\frac{1}{E_1-E_2}\left(\frac{E_2-E_1}{\left(E_1-QHQ\right)\left(E_2-QHQ\right)}\right)QVP \\
= & \quad - \quad PVQ\frac{1}{(E_2-QHQ)^2}QVP.
\end{aligned}$$

With these definitions one can express the potentials R and W in terms of $\hat{Q}$–boxes. Let us classify all contributions to W by a κ number given by

$$\kappa\left(\hat{Q}_{k_1}\ldots\hat{Q}_{k_n}\right) = k_1 + \cdots + k_n. \tag{48}$$

Denote by W_n all $\hat{Q}$-box contributions to W with $\kappa = n$. The potential can be expressed as an infinite sum of those contributions:

$$W = \sum_{n=0}^{\infty} W_n. \tag{49}$$

Here we want to derive explicit expressions for W_0, W_1 and W_2. For this reason let $|\alpha\rangle$ be an eigenstate of PH_0P with an energy E_α from the model space, then the decoupling equation (16) can be written as

$$A|\alpha\rangle = \frac{1}{E_\alpha - QHQ}QVP|\alpha\rangle - \frac{1}{E_\alpha - QHQ}AR|\alpha\rangle. \tag{50}$$

For brevity let us now adopt a notation that whenever a symbol $|\beta\rangle\langle\beta|$ appears the summation over β has to be understood. Now we eliminate A from the potential R:

$$\begin{aligned}
R|\alpha\rangle &= PVP|\alpha\rangle + PVQA|\alpha\rangle \\
&= \hat{Q}(E_\alpha)|\alpha\rangle - PVQ\frac{1}{E_\alpha - QHQ}A|\beta\rangle\langle\beta|R|\alpha\rangle
\end{aligned}$$

$$\begin{aligned}
&= \hat{Q}(E_\alpha)|\alpha\rangle + \hat{Q}_1(E_\alpha, E_\beta)|\beta\rangle\langle\beta|R|\alpha\rangle + PVQ\frac{1}{E_\alpha - QHQ}\frac{1}{E_\beta - QHQ}A|\gamma\rangle\langle\gamma|R|\beta\rangle\langle\beta|R|\alpha\rangle \qquad (51) \\
&= \hat{Q}(E_\alpha)|\alpha\rangle + \hat{Q}_1(E_\alpha, E_\beta)|\beta\rangle\langle\beta|R|\alpha\rangle + \hat{Q}_2(E_\alpha, E_\beta, E_\gamma)|\gamma\rangle\langle\gamma|R|\beta\rangle\langle\beta|R|\alpha\rangle.
\end{aligned}$$

An iterative solution of the previous equation can be given by

$$\begin{aligned} R|\alpha\rangle &= \hat{Q}(E_\alpha)|\alpha\rangle + \hat{Q}_1(E_\alpha,E_\beta)|\beta\rangle\langle\beta|\hat{Q}(E_\alpha)|\alpha\rangle \\ &+ \hat{Q}_1(E_\alpha,E_\beta)|\beta\rangle\langle\beta|\hat{Q}_1(E_\alpha,E_\gamma)|\gamma\rangle\langle\gamma|\hat{Q}(E_\alpha)|\alpha\rangle \\ &+ \hat{Q}_2(E_\alpha,E_\beta,E_\gamma)|\gamma\rangle\langle\gamma|\hat{Q}(E_\beta)|\beta\rangle\langle\beta|\hat{Q}(E_\alpha)|\alpha\rangle + \ldots . \end{aligned} \tag{52}$$

To derive an approximate equation for the operator A we implement the previous equation for R in Eq. (50) and get

$$A|\alpha\rangle = \frac{1}{E_\alpha - QHQ}QVP|\alpha\rangle - \frac{1}{E_\alpha - QHQ}A|\beta\rangle\langle\beta|\hat{Q}(E_\alpha)|\alpha\rangle, \tag{53}$$

where we only take the first term of R , because we are not interested in the calculation of A, but of $A^\dagger A$ (the neglected terms of R would lead to contributions with $\kappa > 2$). The iterative solution of the above equation is given by

$$A|\alpha\rangle = \frac{1}{E_\alpha - QHQ}QVP|\alpha\rangle - \frac{1}{E_\alpha - QHQ}\frac{1}{E_\beta - QHQ}QVP|\beta\rangle\langle\beta|\hat{Q}(E_\alpha)|\alpha\rangle. \tag{54}$$

For the operator $A^\dagger A$ we get

$$\begin{aligned} \langle\delta|A^\dagger A|\alpha\rangle &= -\langle\delta|\hat{Q}_1(E_\delta,E_\alpha)|\alpha\rangle - \langle\delta|\hat{Q}_2(E_\alpha,E_\beta,E_\delta)|\beta\rangle\langle\beta|\hat{Q}(E_\alpha)|\alpha\rangle \\ &- \langle\delta|\hat{Q}(E_\delta)|\beta\rangle\langle\beta|\hat{Q}_2(E_\alpha,E_\beta,E_\delta)|\alpha\rangle. \end{aligned} \tag{55}$$

If we now use the expressions for the operators R and $A^\dagger A$ in Eq. (43) (note that the $\hat{Q}$-box expansion of $A^\dagger A$ starts with a $\hat{Q}_1$-box such that all terms of Eq.(42) with $m+n>2$ lead to contributions with $\kappa > 2$.), we get the following explicit form of W_0, W_1 and W_2:

$$\langle\delta|W_0|\alpha\rangle = \frac{1}{2}\Big\{\langle\delta|\hat{Q}(E_\alpha)|\alpha\rangle + \langle\delta|\hat{Q}(E_\delta)|\alpha\rangle\Big\}, \tag{56}$$

$$\begin{aligned} \langle\delta|W_1|\alpha\rangle &= \frac{1}{2}\Big\{\langle\delta|\hat{Q}_1(E_\alpha,E_\beta)|\beta\rangle\langle\beta|\hat{Q}(E_\alpha)|\alpha\rangle + \langle\delta|\hat{Q}(E_\delta)|\beta\rangle\langle\beta|\hat{Q}_1(E_\beta,E_\delta)|\alpha\rangle\Big\} \\ &+ \frac{1}{8}\Big\{-\langle\delta|\hat{Q}_1(E_\delta,E_\beta)|\beta\rangle\Big(\langle\beta|\hat{Q}(E_\alpha)|\alpha\rangle - \langle\beta|\hat{Q}(E_\beta)|\alpha\rangle\Big) \\ &- \Big(\langle\delta|\hat{Q}(E_\delta)|\beta\rangle - \langle\delta|\hat{Q}(E_\beta)|\beta\rangle\Big)\langle\beta|\hat{Q}_1(E_\beta,E_\alpha)|\alpha\rangle\Big\}, \end{aligned} \tag{57}$$

$$\begin{aligned} \langle\delta|W_2|\alpha\rangle &= \frac{1}{2}\Big\{\langle\delta|\hat{Q}_1(E_\alpha,E_\beta)|\beta\rangle\langle\beta|\hat{Q}_1(E_\alpha,E_\gamma)|\gamma\rangle\langle\gamma|\hat{Q}(E_\alpha)|\alpha\rangle + \langle\delta|\hat{Q}(E_\delta)|\gamma\rangle\langle\gamma|\hat{Q}_1(E_\delta,E_\gamma)|\beta\rangle\langle\beta|\hat{Q}_1(E_\delta,E_\beta)|\alpha\rangle \\ &+ \langle\delta|\hat{Q}_2(E_\alpha,E_\beta,E_\gamma)|\gamma\rangle\langle\gamma|\hat{Q}(E_\beta)|\beta\rangle\langle\beta|\hat{Q}(E_\alpha)|\alpha\rangle + \langle\delta|\hat{Q}(E_\delta)|\beta\rangle\langle\beta|\hat{Q}(E_\beta)|\gamma\rangle\langle\gamma|\hat{Q}_2(E_\delta,E_\beta,E_\gamma)|\alpha\rangle\Big\} \\ &+ \frac{1}{8}\Big\{-\langle\delta|\hat{Q}_1(E_\delta,E_\beta)|\beta\rangle\Big(\langle\beta|\hat{Q}_1(E_\alpha,E_\gamma)|\gamma\rangle\langle\gamma|\hat{Q}(E_\alpha)|\alpha\rangle - \langle\beta|\hat{Q}(E_\beta)|\gamma\rangle\langle\gamma|\hat{Q}_1(E_\beta,E_\gamma)|\alpha\rangle\Big) \\ &- \Big(\langle\delta|\hat{Q}(E_\delta)|\beta\rangle\langle\beta|\hat{Q}_1(E_\delta,E_\beta)|\gamma\rangle - \langle\delta|\hat{Q}_1(E_\gamma,E_\beta)|\beta\rangle\langle\beta|\hat{Q}(E_\gamma)|\gamma\rangle\Big)\langle\gamma|\hat{Q}_1(E_\gamma,E_\alpha)|\alpha\rangle \\ &- \langle\delta|\hat{Q}_2(E_\gamma,E_\beta,E_\delta)|\beta\rangle\langle\beta|\hat{Q}(E_\gamma)|\gamma\rangle\Big(\langle\gamma|\hat{Q}(E_\alpha)|\alpha\rangle - \langle\gamma|\hat{Q}(E_\gamma)|\alpha\rangle\Big) \\ &- \Big(\langle\delta|\hat{Q}(E_\delta)|\beta\rangle - \langle\delta|\hat{Q}(E_\beta)|\beta\rangle\Big)\langle\beta|\hat{Q}_2(E_\alpha,E\gamma,E_\beta)|\gamma\rangle\langle\gamma|\hat{Q}(E_\alpha)|\alpha\rangle \\ &- \langle\delta|\hat{Q}(E_\delta)|\beta\rangle\langle\beta|\hat{Q}_2(E_\gamma,E_\beta,E_\delta)|\gamma\rangle\Big(\langle\gamma|\hat{Q}(E_\alpha)|\alpha\rangle - \langle\gamma|\hat{Q}(E_\gamma)|\alpha\rangle\Big) \\ &- \Big(\langle\delta|\hat{Q}(E_\delta)|\beta\rangle - \langle\delta|\hat{Q}(E_\beta)|\beta\rangle\Big)\langle\beta|\hat{Q}(E_\beta)|\gamma\rangle\langle\gamma|\hat{Q}_2(E_\alpha,E_\gamma,E_\beta)|\alpha\rangle\Big\} \\ &- \frac{1}{16}\Big\{\langle\delta|\hat{Q}_1(E_\delta,E_\beta)|\beta\rangle\langle\beta|\hat{Q}_1(E_\beta,E_\gamma)|\gamma\rangle\Big(\langle\gamma|\hat{Q}(E_\alpha)|\alpha\rangle - \langle\gamma|\hat{Q}(E_\gamma)|\alpha\rangle\Big) \\ &+ \Big(\langle\delta|\hat{Q}(E_\delta)|\beta\rangle - \langle\delta|\hat{Q}(E_\beta)|\beta\rangle\Big)\langle\beta|\hat{Q}_1(E_\beta,E_\gamma)|\gamma\rangle\langle\gamma|\hat{Q}_1(E_\gamma,E_\alpha)|\alpha\rangle\Big\}. \end{aligned} \tag{58}$$

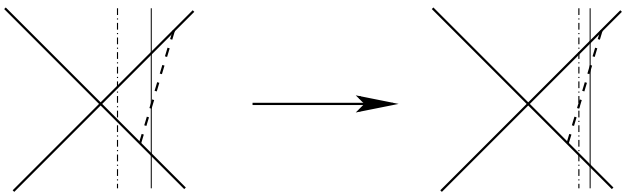

Figure 3: Triangle nucleon–nucleon diagram. The ordinary time-ordered reducible diagram on the left-hand-side becomes an irreducible one by shifting the left (dot-dashed) cut. One gets an irreducible diagram on the right-hand-side with one insertion from a $\hat{Q}_1$-box.

Until now we did not specify the model-space, so the above equation is quite general and can be applied to every problem in chiral perturbation theory with more than one nucleon.

5 Hermitean potential up to a given order

The main advantage of the $\hat{Q}$-box expansion is that it respects the chiral expansion: only a finite number of $\hat{Q}$-boxes contribute to the effective potential up to a given chiral order.

To demonstrate this issue, we fix the model space as consisting of states with two or more nucleons. The states with at least one pion or delta are assumed to belong to the complementary space. Now we can give a diagrammatical interpretation of Eqs. (56), (57) and (58) considering nucleon-nucleon scattering. The interpretation of Eq. (56) is already given in Fig. 2. To give an interpretation of the other two Eqs. (57) and (58) consider first the triangle diagram of Fig. 3. By shifting the NN cut to the $NN\pi$ cut we get an irreducible diagram with one insertion from a $\hat{Q}_1$-box such that this diagram contributes to the term $\langle\delta|\hat{Q}(E_\delta)|\beta\rangle\langle\beta|\hat{Q}_1(E_\beta, E_\delta)|\alpha\rangle$. Even more all possible contributions to $\langle\delta|\hat{Q}(E_\delta)|\beta\rangle\langle\beta|\hat{Q}_1(E_\beta, E_\delta)|\alpha\rangle$ are generated in the same way: every contribution of it can be visualized by a definite diagram with exactly one NN intermediate cut which has to be shifted to the complementary space intermediate states in every possible way. The same is valid for terms including higher $\hat{Q}$-boxes: all contributions of terms with $\kappa = n$ can be visualized by definite diagrams with exactly n NN intermediate cuts, which have to be shifted to the complementary space intermediate states in every possible way.

From this interpretation we see that the higher the κ-number of a $\hat{Q}$-box contribution to the potential W is, the higher is the number of NN cuts which have to be shifted and consequently the higher is the number of loops which increases the chiral order of a given contribution. For this reason there is only a finite number of $\hat{Q}$-box contributions if the chiral order is fixed. Although we restricted here our considerations to nucleon-nucleon scattering, the last statement is quite general: we could choose other model and complementary spaces and show with the same arguments that the $\hat{Q}$-box expansion of the effective potential W stops after a finite number of terms if the chiral order is fixed [#5].

Now we are at the point of showing how one can construct the effective potential W up to given chiral order diagrammatically. The algorithm is indeed very simple:

- Draw all possible covariant diagrams (reducible and irreducible), which contribute up to a given "naive" [#6] chiral order.
- Draw for every covariant diagram all possible time-orderings and classify them by numbers (κ-numbers) of model space intermediate cuts.
- In each time-ordered diagram with $\kappa = n$ shift all n model space intermediate cuts to the complementary space cuts in every possible way. Every diagram generated in this way represents a contribution to a definite $\hat{Q}$-box structure with $\kappa = n$. Summing up all these contributions to the energy propagator we get the irreducible energy denominator of a given time-ordered diagram.
- The energy denominator of a given covariant diagram is then given by the sum of contributions from all possible time-orderings.

[#5] A more formal proof for pion scattering processes off nucleons is presented in the appendix

[#6] By "naive" we mean here that we do not take into account the violation of the power counting by the reducible diagrams.

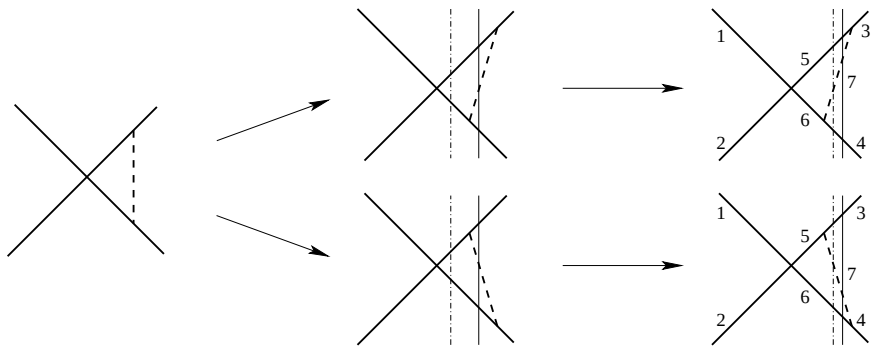

Figure 4: Triangle nucleon-nucleon diagram of chiral order $\nu = 2$. The two steps needed to determine the energy denominator are shown. For the discussion see the main text.

- If $\kappa > 0$ and there are no possibilities to shift the model space intermediate cuts, then the corresponding diagram does not contribute to the effective potential W.

The diagrams constructed according to this procedure obey the power counting, cf. Eq.(6). To make the procedure clear let us discuss some examples:

- The first one is the triangle diagram in nucleon-nucleon scattering shown in Fig. 4. The model space in this case is generated by pure nucleonic states and the complementary space by states with at least one pion or delta. There are only two possible time-ordered diagrams with $\kappa = 1$. The only possibility for shifting the nucleon-nucleon cut is to shift it to the πNN-state (see Fig. 4). All possible contributions to the potential W with $\kappa = 1$ are given in Eq. (57). In this case the states $|\alpha\rangle$, $|\beta\rangle$ and $|\delta\rangle$ denote the two nucleon states $|N_3N_4\rangle$, $|N_5N_6\rangle$ and $|N_1N_2\rangle$, respectively. Consequently

$$E_\alpha = E_3 + E_4, \quad E_\beta = E_5 + E_6, \quad E_\delta = E_1 + E_2. \tag{59}$$

The energy denominators for the upper and lower time-ordered diagrams are given by

$$P_u = -\frac{1}{2}\frac{1}{E_1 + E_2 - E_5 - E_7 - E_4}\frac{1}{E_5 + E_6 - E_5 - E_7 - E_4} \tag{60}$$

and

$$P_l = -\frac{1}{2}\frac{1}{E_1 + E_2 - E_3 - E_7 - E_6}\frac{1}{E_5 + E_6 - E_3 - E_7 - E_6}, \tag{61}$$

respectively. The contribution weighted by 1/8 from Eq. (57) vanishes because the corresponding $\hat{Q}$-box difference is of vertex type:

$$\langle\beta|\hat{Q}(E_\alpha)|\alpha\rangle - \langle\beta|\hat{Q}(E_\beta)|\alpha\rangle = \langle\beta|V|\alpha\rangle - \langle\beta|V|\alpha\rangle + \ldots,$$

where $\langle\beta|V|\alpha\rangle$ denotes the NN vertex. Ellipses denote here terms of higher order, which don't contribute to the considered diagram. The energy denominator P for the covariant triangle diagram is then given by

$$P = P_u + P_l. \tag{62}$$

- As the second example let us consider one-loop pion production diagram shown in Fig. 5. The model space in this case is generated by pure nucleonic states and nucleonic states with one pion or delta. The states including two or more pions or deltas belong now to the complementary space. As we can see from Fig. 5 there are again two time-orderings. The difference to the previous case is that in the upper diagram there are no complementary space intermediate cuts. For this reason the model-space-cuts of the upper diagram can not be shifted and consequently this time-ordered diagram does not contribute to the potential matrix W. In the lower diagram there is a two-nucleon-model-space-cut which can be shifted

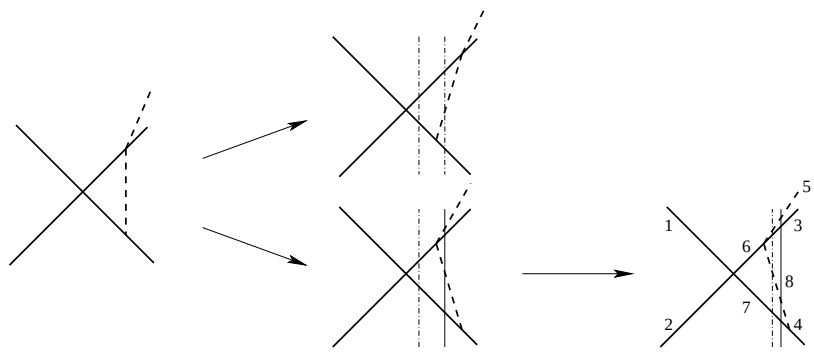

Figure 5: One-loop pion production diagram of chiral order $\nu = 2$. There are two possible time-orderings, which generate 1 diagram by shifting the NN cut to the cut with two pions.

to the two-pion two-nucleon complementary space cut. The only contribution to the energy propagator comes from this diagram. To give the energy denominator we can use Eq. (57), since the κ number of the remaining diagram is equal one:

$$P = -\frac{1}{2}\frac{1}{E_1+E_2-E_5-E_3-E_8-E_7}\frac{1}{E_6+E_7-E_5-E_3-E_8-E_7}. \tag{63}$$

- As the third example let us consider pion production one-loop diagram shown in Fig. 6. In this case there are three time-orderings with $\kappa = 1$ and one time-ordering with $\kappa = 2$. By shifting the model space intermediate cuts we get 6 diagrams with $\kappa = 1$ and one diagram with $\kappa = 2$. To give the energy denominators of the first 6 diagrams with $\kappa = 1$ we can use Eq. (57):

$$\begin{aligned}
P_1 &= -\frac{1}{2}\frac{1}{E_1+E_2-E_1-E_6-E_7-E_4}\frac{1}{E_1+E_2-E_5-E_9-E_7-E_4} \\
&\times \frac{1}{E_8+E_7+E_4-E_5-E_9-E_7-E_4} \\
&+ \frac{1}{8}\frac{1}{E_8+E_7+E_4-E_5-E_9-E_7-E_4}\frac{1}{E_5+E_3+E_4-E_5-E_9-E_7-E_4} \\
&\times \left(\frac{1}{E_1+E_2-E_1-E_6-E_7-E_4} - \frac{1}{E_8+E_7+E_4-E_1-E_6-E_7-E_4}\right), \\
P_2 &= -\frac{1}{2}\frac{1}{E_5+E_3+E_4-E_1-E_6-E_7-E_4}\frac{1}{E_8+E_7+E_4-E_1-E_6-E_7-E_4} \\
&\times \frac{1}{E_5+E_3+E_4-E_5-E_9-E_7-E_4} \\
&+ \frac{1}{8}\frac{1}{E_1+E_2-E_1-E_6-E_7-E_4}\frac{1}{E_8+E_7+E_4-E_1-E_6-E_7-E_4} \\
&\times \left(\frac{1}{E_5+E_3+E_4-E_5-E_9-E_7-E_4} - \frac{1}{E_8+E_7+E_4-E_5-E_9-E_7-E_4}\right), \\
P_3 &= -\frac{1}{2}\frac{1}{E_1+E_2-E_5-E_9-E_6-E_2}\frac{1}{E_1+E_2-E_5-E_9-E_7-E_4} \\
&\times \frac{1}{E_8+E_6+E_2-E_5-E_9-E_7-E_4} \\
P_4 &= -\frac{1}{2}\frac{1}{E_1+E_2-E_5-E_9-E_6-E_2}\frac{1}{E_8+E_6+E_2-E_5-E_9-E_6-E_2} \\
&\times \frac{1}{E_8+E_6+E_2-E_5-E_9-E_7-E_4}
\end{aligned} \tag{64}$$

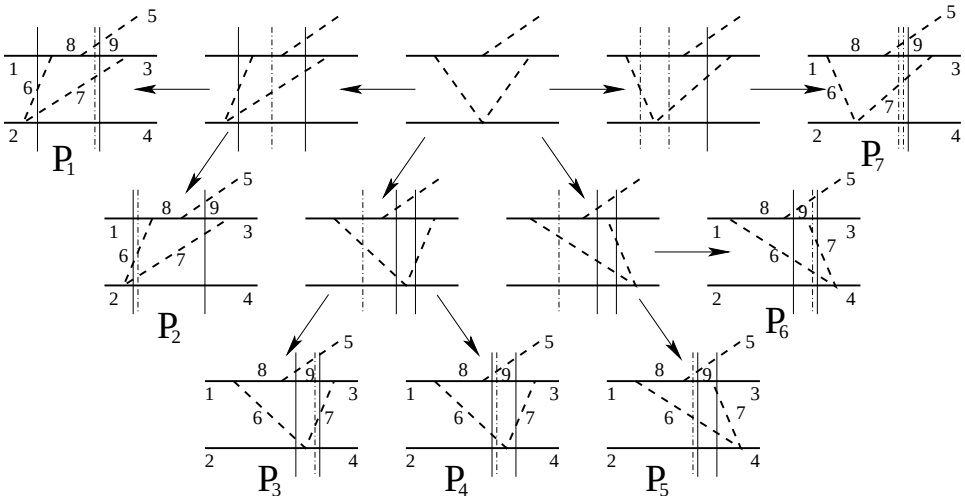

Figure 6: One-loop pion production diagram of chiral order $\nu = 2$ (in standard Weinberg counting). There are four different time-orderings, which generate 7 different diagrams by shifting the πNN intermediate cuts to the cuts with two or more pions.

$$
\begin{aligned}
P_5 &= -\frac{1}{2}\frac{1}{E_1+E_2-E_5-E_9-E_6-E_2}\frac{1}{E_8+E_6+E_2-E_5-E_9-E_6-E_2} \\
&\times \frac{1}{E_8+E_6+E_2-E_5-E_3-E_7-E_6-E_2} \\
P_6 &= -\frac{1}{2}\frac{1}{E_1+E_2-E_5-E_9-E_6-E_2}\frac{1}{E_1+E_2-E_5-E_3-E_7-E_6-E_2} \\
&\times \frac{1}{E_8+E_6+E_2-E_5-E_3-E_7-E_6-E_2}
\end{aligned}
$$

$$
\begin{aligned}
P_7 &= \frac{1}{2}\frac{1}{E_1+E_2-E_5-E_9-E_7-E_4}\frac{1}{E_8+E_6+E_2-E_5-E_9-E_7-E_4} \\
&\times \frac{1}{E_8+E_7+E_4-E_5-E_9-E_7-E_4}
\end{aligned} \tag{65}
$$

The whole energy denominator is then given by a sum of all seven contributions:

$$P = P_1 + \cdots + P_7. \tag{66}$$

To give the expression for P_7 we used Eq. (58) for the $\kappa = 2$ contribution to W. Note that there are no contributions to P_7 weighted by 1/8 and 1/16, since the corresponding $\hat{Q}$-box differences are of vertex type.

From the third example we see that the expressions for the energy denominators can be rather lengthy. For this reason it might be nice to have an independent check of them. This indeed can be easily done: If one requires the on-shell condition (the initial and final energy of a given scattering process are required to be equal), then every time-ordered diagram (reducible or irreducible) can be written in terms of hermitean potentials, including some iterations from the Lippman-Schwinger equation. This is illustrated in Fig. 7 for the one-loop reducible triangle nucleon-nucleon scattering diagram. The corresponding potentials are denoted by a gray shaded area. The energy denominators of both diagrams, the first one (which comes from the first iteration in the Lippman-Schwinger equation) composed of two contributions and the second one composed of one contribution from the hermitean potential, are given by

$$T_1 = \frac{1}{E-E_5-E_6}\frac{1}{2}\left(\frac{1}{E_5+E_6-E_5-E_7-E_4}+\frac{1}{E-E_5-E_7-E_4}\right) \tag{67}$$

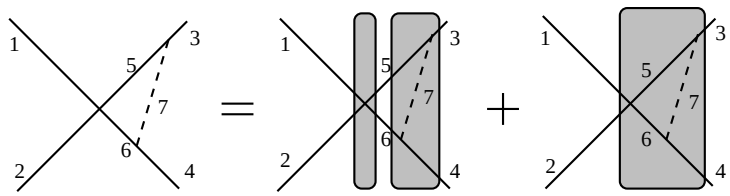

Figure 7: One-loop triangle nucleon-nucleon time-ordered diagram written in terms of hermitean potentials denoted by gray shaded area.

and

$$T_2 = -\frac{1}{2}\frac{1}{E - E_5 - E_7 - E_4}\frac{1}{E_5 + E_6 - E_5 - E_7 - E_4}, \tag{68}$$

respectively. Here we use the on shell condition $E = E_1 + E_2 = E_3 + E_4$. If we now sum up the two contributions T_1 and T_2 we get the familiar energy denominator of the corresponding time-ordered diagram[#7]:

$$T_1 + T_2 \quad = \quad \frac{1}{E - E_5 - E_6}\frac{1}{E - E_5 - E_7 - E_4}. \tag{69}$$

In the same way one should be able to reconstruct every possible time-ordered diagram.

6 Some leading order considerations

Let us briefly discuss the differences between some hermitean and non-hermitean potentials in the case of pion scattering on few-nucleon systems. We denote the corresponding potentials here by W and W', respectively. Let us now consider some diagrams, which contribute to the potentials W or W' at leading order in the $1/m$ expansion, namely in the static limit $m \to \infty$. If we assume that the incoming and outgoing pions of the potentials W or W' are not involved in further interactions in the kernel, then (because of the on-shell condition) their energies have to be equal in the static limit. In this case contributions to the potential W' can be identified with the $\kappa = 0$ contributions to W. All other contributions to W with $\kappa > 0$ are called Okubo-type corrections (these corrections are also called wave function orthonormalization diagrams [24]). In some cases

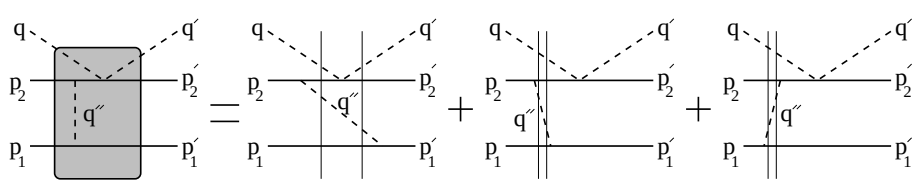

Figure 8: Time-ordered diagram with two Okubo-type corrections for pion scattering off two nucleons.

the Okubo-type corrections cancel some time-ordered diagrams from W'. Consider e.g. the pion scattering diagrams shown in Fig. 8. The first time-ordered diagram contributes obviously to W and W'. The two other diagrams are Okubo-type corrections. The energy denominators of these three diagrams are given by

$$P_1 = \frac{1}{E_{q''}^2}\ , \quad P_2 = -\frac{1}{2}\frac{1}{E_{q''}^2}\ , \quad P_3 = -\frac{1}{2}\frac{1}{E_{q''}^2}\ , \tag{70}$$

such that their sum cancels. Here $E_{q''}$ denotes the energy of the rescattered pion. The same happens if we consider the pion-scattering diagrams on three nucleons, shown in Fig. 9. The Okubo-corrections cancel again the time-ordered diagram. Like in the case of three nucleon scattering [1, 25, 24, 7] it is straightforward to see that the contributions to W in the case of pion scattering on three nucleons, shown in Fig. 10, vanish.

[#7]Note that this calculation serves only to check the correctness of energy denominators in the effective potential. A strictly perturbative approach makes no sense in the case of nucleon-nucleon scattering.

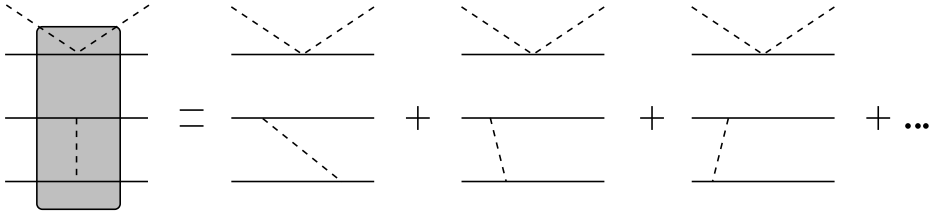

Figure 9: Pion scattering on three nucleons: time-ordered diagram with two Okubo-type corrections. The ellipses denote the other time-ordered diagram with the corresponding Okubo-type correction.

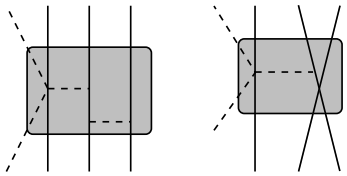

Figure 10: Two diagrams that contribute to the hermitean potential in the case of pion scattering off three nucleons.

Acknowledgements

We are grateful to Evgeny Epelbaum for his numerous useful comments.

A The degenerate case

The aim of the three following appendices is to give the formal proof that the $\hat{Q}$-box contributions with $\kappa > 2$ (see Eq. (48)) lead in the case of pure nucleonic scattering to operators of chiral orders $\nu > 10 - 3N$ and in the case of pion scattering off nucleons to operators of chiral orders $\nu > 7 - 3N$. Such kind of operators contribute in the case of pure nucleonic scattering to the orders higher than NNNLO. In the case of pion scattering on nucleons they lead to the kernel contributions of order higher than $\mathcal{O}(q^4)$ in the conventional counting, see e.g. [26] for a detailed discussion.

Let us assume for the moment that all states from the model-space have the same energy E. In this case we can express the potentials R and W in terms of $\hat{Q}$-boxes in a compact way. The operator PH_0P can now be replaced by EP and the higher $\hat{Q}$-boxes by

$$\begin{aligned} \hat{Q}_n &= \frac{1}{n!}\frac{d^n\hat{Q}}{dE^n} \\ &= (-1)^n PVQ\left(\frac{1}{E-QHQ}\right)^{n+1} QVP. \end{aligned} \tag{A.1}$$

The decoupling equation (16) for the operator A becomes

$$A = \frac{1}{E-QHQ}QVP - \frac{1}{E-QHQ}AR, \tag{A.2}$$

with R as given in the Eq. (31)

$$R = PVP + PVQA.$$

Eliminating A from both equations above and using the definition of $\hat{Q}_n$ we obtain

$$R = \sum_{n=0}^{\infty}\hat{Q}_n R^n, \tag{A.3}$$

where we have used the notation $\hat{Q}_0 = \hat{Q}$ for $n = 0$. This equation can be solved exactly as [13]

$$R = \sum_{k=1}^{\infty} \sum_{m_1,...,m_k} f(m_1,...,m_k)\hat{Q}_{m_1} \cdots \hat{Q}_{m_k}. \tag{A.4}$$

The $f(m_1,...,m_k)$ are coefficients defined by

$$f(m_1,...,m_k) = \begin{cases} \delta_{m_1,0} & \text{for } k = 1 \\ \delta_{m_2,0}\delta_{m_1,1} & \text{for } k = 2 \\ \delta_{m_k,0}\delta_{m_1+\cdots+m_k,k-1} \prod_{i=1}^{k-2} \theta\left(i - \sum_{j=1}^{i} m_{k-j}\right) & \text{for } k \geq 3, \end{cases} \tag{A.5}$$

where $\theta(x)$ is the step function

$$\theta(x) = \begin{cases} 1 & \text{for } x \geq 0 \\ 0 & \text{for } x < 0. \end{cases} \tag{A.6}$$

Let us introduce a convenient notation for representing the series of R. We define a symbol $[m]_k$, which denotes a set of k elements which are zero or a positive integer

$$[m]_k = (m_1,...,m_k). \tag{A.7}$$

We further define

$$\hat{Q}[m]_k = \hat{Q}_{m_1} \cdots \hat{Q}_{m_k}. \tag{A.8}$$

Using these simple notations, we may write R as

$$R = \sum_{k=1}^{\infty} \sum_{[m]_k} f([m]_k)\hat{Q}[m]_k. \tag{A.9}$$

The coefficient $f([m]_k)$ has an interesting property:

$$f([m]_{k_1}) \cdots f([m]_{k_n}) = f(n, [m]_{k_1}, ..., [m]_{k_n}), \tag{A.10}$$

such that the operator R^n can be written as

$$R^n = \sum_{k=0}^{\infty} \sum_{[m]_k} f(n, [m]_k)\hat{Q}[m]_k, \tag{A.11}$$

where we use the notation

$$f(n, [m]_0) = f(n). \tag{A.12}$$

Now we can solve Eq. (A.2) for A exactly: iterating Eq. (A.2) we have

$$A = \sum_{n=0}^{\infty} (-1)^n \left(\frac{1}{E - QHQ}\right)^{n+1} QVPR^n \tag{A.13}$$

$$= \sum_{n=0}^{\infty} \sum_{k=0}^{\infty} \sum_{[m]_k} (-1)^n f(n, [m]_k) \left(\frac{1}{E - QHQ}\right)^{n+1} QVP\hat{Q}[m]_k. \tag{A.14}$$

Multiplication with $A^\dagger$ gives

$$A^\dagger A = -\sum_{p=0}^{\infty} \sum_{q=0}^{\infty} \sum_{k=0}^{\infty} \sum_{l=0}^{\infty} \sum_{[m]_k} \sum_{[n]_l} f(p, [m]_k) f(q, [n]_l) \hat{Q}^\dagger [m]_k \hat{Q}_{p+q+1} \hat{Q}[n]_l. \tag{A.15}$$

Therefore, we can write $A^\dagger A$ as a sum of definite combinations of $\hat{Q}$-boxes. We see from the above equation that the coefficients in front of the $\hat{Q}$-box combinations in the sum have the value 0 or 1. They serve to exclude all impossible $\hat{Q}$-box combinations. From the definition of the function f in Eq. (A.5) we see, that the coefficients in the sum of Eq. (A.15) are zero unless

$$p + m_1 + \cdots + m_k \;=\; k \quad \text{and} \quad q + n_1 + \cdots + n_l \;=\; l \tag{A.16}$$

If we write $A^\dagger A$ as

$$A^\dagger A \;=\; -\sum_{r=1}^{\infty} \sum_{[m]_r} h([m]_r) \hat{Q}[m]_r, \tag{A.17}$$

we obtain that the coefficients $h([m]_r)$ are zero unless $m_1 + \cdots + m_r = r$. This and the similar property of the coefficients $f([m]_r)$, namely they are zero unless $m_1 + \cdots + m_{r-1} = r - 1$ and $m_r = 0$, will play an important role for the later power counting arguments.

B Power counting for $\hat{Q}$-boxes

Let us derive the power counting for the $\hat{Q}(E)$-box following Weinberg's arguments. A general time-ordered diagram of the $\hat{Q}$-box has the following form:

$$\int (d^3q)^L \frac{1}{(E_k - E_l)^R} \left(\frac{1}{\sqrt{2E_\pi}} \right)^{2I_p} \prod_i q^{d_i V_i}$$

where L is the number of loops, R is the number of energy-denominators, d_i is the dimension of a vertex i and V_i counts how often the vertex of type i appears in the diagram. Under I_p, E_p, I_n and E_n we understand the number of inner pion, external pion, inner nucleon and external nucleon-lines. For the chiral order ν one gets

$$\nu \;=\; 3L - R - I_p + \sum_i V_i d_i - 3(C + D_p + D_n - 1), \tag{B.18}$$

where C, D_p and D_n denote the number of connected, disconnected pion (pion spectators) and disconnected nucleon (nucleon spectators) pieces, respectively. Each connected and disconnected piece brings a delta function, which carries dimension -3. The overall delta function is not taken into account, for this reason $(C+D_p+D_n-1)$ appears in the above equation. The phase-factors $1/\sqrt{2E_\pi}$ of external pions are also not taken into account. With the help of the topological identities

$$\sum_i V_i n_i \;=\; 2I_n + E_n - 2D_n, \tag{B.19}$$

$$\sum_i V_i p_i \;=\; 2I_p + E_p - 2D_p, \tag{B.20}$$

and

$$L \;=\; C + I_p + I_n - \sum_i V_i, \tag{B.21}$$

$$R \;=\; \sum_i V_i - 1, \tag{B.22}$$

we get the master formula[#8]

$$\nu \;=\; 4 - 3N - D_p - E_p + \sum_i V_i \kappa_i, \tag{B.23}$$

[#8] For $D_p = 0$ one can easily verify that the equations (B.23) and (6) are identical.

where

$$\kappa_i = d_i + \frac{3}{2}n_i + p_i - 4, \tag{B.24}$$

and n_i denotes the number of nucleons in vertex i, which can only be even, and p_i counts the number of pion fields associated to the vertex i.

In the case of the nucleon-nucleon interaction there are no external pions so that $D_p = E_p = 0$ and we get a simplified formula for the chiral order

$$\nu = 4 - 3N + \sum_i V_i \kappa_i. \tag{B.25}$$

Because of chiral symmetry, κ_i has to be a positive number, thus the order of every diagram is bounded from below. The lowest possible order for a $\hat{Q}$-box is $\nu_{\min} = 6 - 3N$ and is represented through the lowest contact term from $\mathcal{L}^{(0)}_{NN}$ or the pion exchange diagram with the vertices from $\mathcal{L}^{(1)}_{\pi N}$. We understand from now on the $\hat{Q}$-box as organized in a chiral expansion,

$$\hat{Q}(E) = \sum_{i=0}^{\infty} \hat{Q}^{(6-3N+i)}(E), \tag{B.26}$$

where the upper index denotes the chiral order. Analogously we can write the higher $\hat{Q}$-boxes as

$$\hat{Q}_n(E_1, ..., E_{n+1}) = \sum_{i=0}^{\infty} \hat{Q}_n^{(6-3N-n+i)}(E_1, ..., E_{n+1}), \tag{B.27}$$

with

$$\hat{Q}_n^{(6-3N-n+i)}(E_1, ..., E_{n+1}) = \sum_{k=1}^{n+1} C_k(E_1, ..., E_{n+1}) \hat{Q}^{(6-3N+i)}(E_k), \tag{B.28}$$

where $C_k(E_1, ..., E_{n+1})$ is defined in Eq. (47). The following combination of $\hat{Q}$-boxes

$$\begin{aligned} \hat{O} &= \hat{Q}_n^{(6-3N-n+i)}(E_{1,1}, ..., E_{1,n+1}) \hat{Q}_m^{(6-3N-m+j)}(E_{2,1}, ..., E_{2,m+1}) \\ &= \hat{Q}_n^{(6-3N-n+i)}(E_{1,1}, ..., E_{1,n+1}) |\alpha\rangle\langle\alpha| \hat{Q}_m^{(6-3N-m+j)}(E_{2,1}, ..., E_{2,m+1}) \end{aligned}$$

leads to the chiral order $\nu(\hat{O})$:

$$\begin{aligned} \nu(\hat{O}) &= 6 - 3N - n + i + 6 - 3N - m + j + 3(N-1) \\ &= 9 - 3N + i + j - n - m, \end{aligned} \tag{B.29}$$

where the factor $3(N-1)$ comes from the integration over all relative coordinates of the intermediate state $|\alpha\rangle\langle\alpha|$. For a general combination of $\hat{Q}$-boxes

$$\hat{O} = \hat{Q}_{n_1}^{(6-3N-n_1+i_1)}(E_{1,1}, ..., E_{1,n_1+1}) \cdots \hat{Q}_{n_m}^{(6-3N-n_m+i_m)}(E_{m,1}, ..., E_{m,n_m+1})$$

we get

$$\begin{aligned} \nu(\hat{O}) &= m(6-3N) - (n_1 + ... + n_m) + (i_1 + ... + i_m) + (m-1)3(N-1) \\ &= 3m + 3 - 3N - (n_1 + ... + n_m) + (i_1 + ... + i_m). \end{aligned} \tag{B.30}$$

Now we are ready to proof that one can neglect higher $\hat{Q}$-boxes for the case of pure nucleonic scattering. At the first sight it is not clear, why the $\hat{Q}$-box contributions with increasing κ number should increase the chiral order. Conversely, we see from the last equation that the order $\nu(\hat{O})$ decreases with increasing $\kappa = n_1 + \cdots + n_m$. To clarify this we first point out that the steps for the derivation of the operators R and $A^\dagger A$ in the degenerate and in the non-degenerate case were the same. The coefficients in front of the $\hat{Q}$-boxes are the same, the difference is only in the energy-structure of the $\hat{Q}$-boxes. From the degenerate case we learned

that the coefficients $f(n_1, ..., n_m)$ and $h(n_1, ..., n_m)$ of the operators R and $A^\dagger A$ restrict the numbers $n_1, ..., n_m$, namely $f(n_1, ..., n_m) \neq 0$ only if the condition $n_1 + ... + n_m = m - 1$ is valid and $h(n_1, ..., n_m) \neq 0$ only if the condition $n_1 + ... + n_m = m$ is valid. As a result we get for the operator R that

$$n_1 + ... + n_m \quad = \quad m - 1 \tag{B.31}$$

and from Eq. (B.30)

$$\begin{aligned} \nu(\hat{O}) &= 3m + 3 - 3N - m + 1 + (i_1 + ... + i_m) \\ &= 2m + 4 - 3N + (i_1 + ... + i_m). \end{aligned}$$

The NNNLO will be reached when $\nu = 10 - 3N$. One obtains from the above equation that $m \leq 3$ and $\kappa = n_1 + ... + n_m \leq 2$. All the other possibilities are beyond NNNLO. For the operator $A^\dagger A$ we get

$$n_1 + ... + n_m \quad = \quad m.$$

However, we have to remember that the operator $A^\dagger A$ appears in the hermitean potential W only in combination with the operator R, which can be directly seen from Eq. (42). For this reason a $\hat{Q}$-box combination $\hat{Q}_{n_1} \cdots \hat{Q}_{n_m}$ from $A^\dagger A$ has to be multiplied by the $\hat{Q}$-box combination $\hat{Q}_{l_1} \cdots \hat{Q}_{l_k}$ from R. So for the whole operator we get $n_1 + ... + n_m = m$ and $l_1 + ... + l_k = k - 1$ and altogether

$$\kappa = n_1 + ... + n_m + l_1 + ... + l_k = m + k - 1. \tag{B.32}$$

From the above considerations we see, that the condition $m + k \leq 3$ has to be valid. With similar arguments one can show that the operators of the form

$$\left(A^\dagger A\right)^m R \left(A^\dagger A\right)^n \tag{B.33}$$

with $m + n > 2$ contribute to orders higher than $10 - 3N$.

C Power counting for pion scattering on nucleons

In this section we want to consider the scattering of pions off nucleons, so we define our model-space as a space, which contains the states with only nucleons and nucleon states with at least one pion or delta. The states with more than two pions are in the complementary space. The power counting of Weinberg given in Eq. (B.23) remains the same but D_p and E_p do not vanish any more, because external pions can appear.

We have again to prove the assumption that one can neglect the higher $\hat{Q}$-boxes for this kind of processes. For this reason let us introduce a convenient notation: we write the projection operator P as $P = P^0 + P^1$, where P^0 and P^1 project to the pure nucleonic states and nucleonic states with one pion. Utilizing this notation one can write a $\hat{Q}$-box as a two–by–two matrix:

$$\begin{pmatrix} P^1\hat{Q}(E)P^1 & P^1\hat{Q}(E)P^0 \\ P^0\hat{Q}(E)P^1 & P^0\hat{Q}(E)P^0 \end{pmatrix} . \tag{C.34}$$

The multiplication of $\hat{Q}$-boxes is nothing but a matrix multiplication. At this stage there appears one problem: in the power counting Eq. (6) we did not count the phase-space factors of external pions. However, when we construct a $\hat{Q}$-box we a priori do not know whether the outgoing pions of the box are internal or external. Indeed the assumption that all outgoing pion lines of a $\hat{Q}$-box are external results in a contradiction, because by multiplication of two $\hat{Q}$-boxes external pion lines can become internal. For this reason let us introduce some kind of internal power counting, where we count all phase-space factors of pions, and denote the internal chiral order as $\tilde{\nu}$. The number of phase-space factors of external pions is given by $E_p - 2D_p$. We get the internal order by simply subtracting the factor $(E_p/2 - D_p)$ from the original order:

$$\tilde{\nu} \quad = \quad \nu - \frac{E_p}{2} + D_p \; = \; 4 - 3N - \frac{3}{2}E_p + \sum_i V_i \kappa_i \tag{C.35}$$

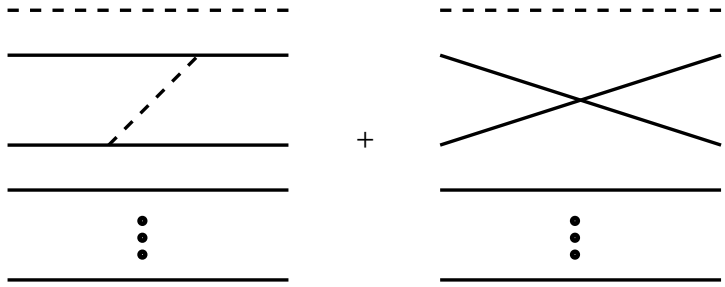

Figure 11: $P^1\hat{Q}(E)P^1$-boxes to leading order.

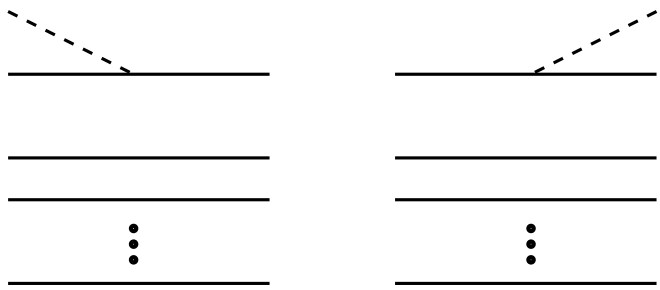

Figure 12: $P^1\hat{Q}(E)P^0$ and $P^0\hat{Q}(E)P^1$-boxes to leading order.

Every matrix-element has its definite minimal original and internal order. The minimal internal order of $P^1\hat{Q}(E)P^1$ is $\tilde{\nu}_{\min} = 3 - 3N$ and is represented by the diagrams of Figure 11. The lowest internal orders of elements $P^0\hat{Q}(E)P^1$ and $P^1\hat{Q}(E)P^0$ is $\tilde{\nu}_{\min} = 3 - 3N + 1/2$ and is represented by the diagrams of Figure 12. Finally the lowest internal order of elements $P^0\hat{Q}(E)P^0$ is given by $\tilde{\nu}_{\min} = 6 - 3N$ and is represented through the contact interaction. All the vertices in the above mentioned diagrams stem from $\mathcal{L}^{(1)}_{\pi N}$ and $\mathcal{L}^{(0)}_{NN}$. To have an overview let us define an order matrix as

$$\tilde{\nu}\begin{pmatrix} P^1\hat{Q}(E)P^1 & P^1\hat{Q}(E)P^0 \\ P^0\hat{Q}(E)P^1 & P^0\hat{Q}(E)P^0 \end{pmatrix} = \begin{pmatrix} \tilde{\nu}(P^1\hat{Q}(E)P^1) & \tilde{\nu}(P^1\hat{Q}(E)P^0) \\ \tilde{\nu}(P^0\hat{Q}(E)P^1) & \tilde{\nu}(P^0\hat{Q}(E)P^0) \end{pmatrix}. \tag{C.36}$$

With this notation we have for the minimal internal chiral order of $\hat{Q}$-boxes

$$\tilde{\nu}_{\min}\begin{pmatrix} P^1\hat{Q}(E)P^1 & P^1\hat{Q}(E)P^0 \\ P^0\hat{Q}(E)P^1 & P^0\hat{Q}(E)P^0 \end{pmatrix} = \begin{pmatrix} 3-3N & 3-3N+\frac{1}{2} \\ 3-3N+\frac{1}{2} & 6-3N \end{pmatrix} \tag{C.37}$$

and for higher $\hat{Q}$-boxes

$$\begin{aligned} \hat{O} &= \begin{pmatrix} P^1\hat{Q}_n(E_1,...,E_{n+1})P^1 & P^1\hat{Q}_n(E_1,...,E_{n+1})P^0 \\ P^0\hat{Q}_n(E_1,...,E_{n+1})P^1 & P^0\hat{Q}_n(E_1,...,E_{n+1})P^0 \end{pmatrix} \\ \tilde{\nu}_{\min}(\hat{O}) &= \begin{pmatrix} 3-3N-n & 5-3N+\frac{1}{2}-n \\ 5-3N+\frac{1}{2}-n & 8-3N-n \end{pmatrix}, \end{aligned} \tag{C.38}$$

where $n \geq 1$. The maximal order, which corresponds to order q^4 in pion scattering off nucleons (standard single-nucleon counting) is given by $\nu_{\max} = 7 - 3N$. The following matrix of $\hat{Q}$-boxes

$$\begin{pmatrix} P^1\hat{Q}_n^{(3-3N-n+j)}(E_1,...,E_{n+1})P^1 & P^1\hat{Q}_n^{(3-3N+\frac{1}{2}-n+j)}(E_1,...,E_{n+1})P^0 \\ P^0\hat{Q}_n^{(3-3N+\frac{1}{2}-n+j)}(E_1,...,E_{n+1})P^1 & P^0\hat{Q}_n^{(6-3N-n+j)}(E_1,...,E_{n+1})P^0 \end{pmatrix}$$

can also be represented as

$$P^{i_1}\hat{Q}_n^{(5-\frac{3}{2}(i_1+i_2)+\delta_{i_1,i_2}-3N-n+j)}(E_1,...,E_{n+1})P^{i_2}.$$

For the order of m multiplied $\hat{Q}$-boxes

$$\begin{aligned}\hat{O} &= P^{i_1}\hat{Q}_{n_1}^{(5-\frac{3}{2}(i_1+i_2)+\delta_{i_1,i_2}-3N-n_1+j_1)}(E_{1,1},...,E_{1,n_1+1})P^{i_2}\\ ... &\quad P^{i_m}\hat{Q}_{n_m}^{(5-\frac{3}{2}(i_m+i_{m+1})+\delta_{i_m,i_{m+1}}-3N-n_m+j_m)}(E_{m,1},...,E_{m,n_m+1})P^{i_{m+1}}\end{aligned}$$

we get

$$\begin{aligned}\tilde{\nu}(\hat{O}) &= m(5-3N)-(n_1+...+n_m)+(j_1+...+j_m)+(m-1)3N\\ &- \frac{3}{2}(i_1+i_{m+1})+\sum_{k=1}^{m}\delta_{i_k,i_{k+1}}-3(i_2+...+i_m)-3\sum_{k=2}^{m}\delta_{i_k,0}.\end{aligned} \tag{C.39}$$

The last sum of Kronecker-symbols comes from the integration over the intermediate states. The integration over the relative coordinates brings in the case of a pure nucleonic intermediate state $3(N-1)$ and in the case of a state with one pion $3N$ extra dimensions in the power counting. For the construction of the operator R we can use the following relations

$$\begin{aligned}m-1 &= n_1+..+.n_m,\\ m-1 &= i_2+...+i_m+\sum_{k=2}^{m}\delta_{i_k,0},\end{aligned}$$

where the fact that $i_2,...,i_m\in\{0,1\}$ has been used, and we get for the internal order

$$\begin{aligned}\tilde{\nu}(\hat{O}) &= m-3N+4+\left(\sum_{k=1}^{m}\delta_{i_k,i_{k+1}}-\frac{3}{2}i_1-\frac{3}{2}i_{m+1}\right)+(j_1+...+j_m)\\ &\geq m-3N+1,\end{aligned} \tag{C.40}$$

such that the relation $m\leq 6$ has to hold. However, the value of m can be further decreased. The above inequality becomes an equality, if $i_1=i_{m+1}=1$ and the sum of the Kronecker-symbols is zero. Let us discuss first this elastic case. For every $k=1,...,m$ the condition $i_k\neq i_{k+1}$ is valid. In this case at least one pure nucleonic intermediate state has to appear. It follows that $D_p=0$ and the original order of this combination of $\hat{Q}$-boxes is $\nu=\tilde{\nu}+E_p/2=m-3N+2$ leading to the condition $m\leq 5$. In the inelastic case $i_1=0$ or $i_{m+1}=0$ the original order is given by $\nu\geq m-3N+3$, such that even the condition $m\leq 4$ has to be valid. Further decreasing of m will be obtained in the following manner: let us assume the equality $m=5$. In the elastic case $i_1=i_{m+1}=1$ the condition $\sum_{k=1}^{m}\delta_{i_k,i_{k+1}}\leq 1$ has to be valid. For $m=5$ only the equality is possible, so that there appears at least one pure nucleonic intermediate state and the original order increases by one, such that $\nu=8-3N$ and is beyond the fourth order. In the inelastic case the condition $m=5$ is excluded and we get $m\leq 4$. Let us assume that $m=4$. In the elastic case we get the condition $\sum_{k=1}^{m}\delta_{i_k,i_{k+1}}\leq 2$. In any case one pure intermediate nucleonic state has to appear, otherwise we would get $\sum_{k=1}^{m}\delta_{i_k,i_{k+1}}=4$. This restricts the above estimation to $\sum_{k=1}^{m}\delta_{i_k,i_{k+1}}\leq 1$. For $m=4$ only the equality $\sum_{k=1}^{m}\delta_{i_k,i_{k+1}}=0$ is possible with the $\hat{Q}$-box combination given by $P^1\hat{Q}_{n_1}P^0\hat{Q}_{n_2}P^1\hat{Q}_{n_3}P^0\hat{Q}_{n_4}P^1$. However, for $m=4$ at least one higher $\hat{Q}$-box has to appear. For the above combination of $\hat{Q}$-boxes one gets an increase of the original order by two, such that $\nu=8-3N$. In the inelastic case we get the condition $\sum_{k=1}^{m}\delta_{i_k,i_{k+1}}=0$, which is impossible for $m=4$. This proves that the $\hat{Q}$-box contributions to R with $\kappa>2$ are of higher order than $7-3N$, that is they start to contribute at $\mathcal{O}(q^5)$ in the standard single–nucleon counting. The proof that the operators

$$\left(A^\dagger A\right)^m R\left(A^\dagger A\right)^n \tag{C.41}$$

are of higher order than $7-3N$ if $m+n>2$ can be given in the similar manner (the same holds for the $\kappa>2$ contributions if $m+n\leq 2$).

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