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Block-diagonal similarity renormalization group and effective nucleon-nucleon interactions

S. Szpigel[1], V. S. Timóteo[2] and E. Ruiz Arriola[3]

[1] Centro de Rádio-Astronomia e Astrofísica Mackenzie, Universidade Presbiteriana Mackenzie
01302-907, São Paulo, SP, Brasil
[2] Grupo de Óptica e Modelagem Numérica - GOMNI, Universidade Estadual de Campinas
13484-332, Limeira, SP, Brasil
[3] Departments de Física Atómica, Molecular y Nuclear, Universidad de Granada
E-18071, Granada, Andalucia, España

E-mail: E-mail: szpigel@mackenzie.br (SS)

E-mail: E-mail: varese@ft.unicamp.br (VST)

E-mail: E-mail: earriola@ugr.es (ERA)

Abstract. We apply the block-diagonal similarity renormalization group to a simple toy-model for the nucleon-nucleon (NN) interaction in the ${}^1S_0$ channel, aiming to analyze the complementarity between the explicit and the implicit renormalization approaches in nuclear physics. By *explicit* renormalization we mean the methods based on the wilsonian renormalization group in which high-energy modes above a given cutoff scale are integrated out while their effects are replaced by scale dependent effective interactions consistently generated in the process. We call *implicit* renormalization the usual procedure of cutoff effective theories in which the high-energy modes above the cutoff scale are simply removed and their effects are included through parametrized cutoff dependent counterterms whose strengths are fixed by fitting low-energy data. We compare the effective interactions obtained in both schemes and find a wide range of cutoff scales where they overlap. We further analyze the role played by the one-pion exchange (OPE) considering a δ-shell plus OPE representation for the NN interaction.

1. Introduction
The idea of effective interactions has been strongly pursued since the late 1950s after the pioneering works by Goldstone [1], Moshinsky [2] and Skyrme [3], who suggested to use this notion to overcome the complications which appear in the solution of the nuclear many-body problem due to the large short-range repulsive core. This allowed to take advantage of the much simpler mean field framework based on those effective interactions in the implementation of nuclear structure calculations [4]. The main problem of the effective interaction approach is both the proliferation of independent parameters as well as their huge numerical diversity [5]. This reflects both the lack of an unambiguous link to the fundamental nucleon-nucleon (NN) interaction as well as the quite disparate finite nuclei and nuclear matter observables which have been used to fix the effective theory parameters. In recent works [6, 7] an effort has been made in order to understand the origin of the NN effective interactions from free space NN scattering in a model independent way, without invoking finite nuclei nor nuclear matter properties. This approach corresponds to what will be called here as *implicit* renormalization.

An intense reformulation of the nuclear many-body problem has taken place in the last ten years inspired by the wilsonian renormalization group ideas, providing an alternative approach to the determination of effective interactions directly from the NN *bare* potentials fitted to the scattering data (for reviews see e.g. [8, 9, 10] and references therein). The basis of the whole approach is to take advantage of choosing the proper resolution scale in the formulation of the problem, separating explicitly what degrees of freedom and interactions behave dynamically below that scale. This approach corresponds to what will be called here as *explicit* renormalization. Within this framework, the so called $V_{\text{low k}}$ approach [11] has been used to consistently integrate out the high-momentum components of both high-precision [12, 13] and chiral effective field theory (ChEFT) [14, 15] NN potentials in order to derive phase-shift equivalent softer forms. A more recent approach that has been applied in this context is the similarity renormalization group (SRG), which provides a great deal of simplification in the derivation of effective interactions for many-body calculations in nuclear physics [16]. The basic strategy underlying the application of the SRG methods to nuclear forces is to evolve the initial *bare* potential via a continuous unitary transformation that runs a cutoff λ on energy differences. Such a transformation generates a family of unitarily equivalent smooth interactions $H_\lambda = U_\lambda \, H \, U_\lambda^\dagger$ with a band-diagonal structure of a prescribed width roughly given by the SRG cutoff λ. One of the main advantages of the SRG method over the $V_{\text{low k}}$ is that it allows for a straightforward and consistent treatment of the scale dependence of induced as well as initially introduced many-body forces [17].

In this contribution we present a summary of previous works [18, 19, 20] where we have applied the block-diagonal similarity renormalization group (BD-SRG) scheme [21] to the NN system. We considered a simple toy-model for the NN interaction in the $^1S_0$ and $^3S_1$ partial-wave channels, which is constructed such that the phase-shifts at low-momenta and the deuteron binding-energy are reasonably described with a short-range interaction and makes the SRG evolution towards small values of the SRG cutoff λ much more practical. As we have shown, the BD-SRG allows to implement a block-diagonal separation of the Hilbert space in two orthogonal (decoupled) subspaces, $\mathcal{H} = \mathcal{H}_P \oplus \mathcal{H}_Q$, which are respectively below or above a cutoff scale Λ, which will be referred as the block-diagonal (BD) cutoff. The unitary evolution runs the SRG cutoff from $\lambda \to \infty$ (the ultraviolet limit) to $\lambda \to 0$ (the infrared limit) and interpolates between the initial *bare* hamiltonian $H \equiv H_{\lambda \to \infty}$ and the block-diagonal one $H_{\lambda \to 0}$. This corresponds to a unitary implementation to all energies of the $V_{\text{low k}}$ approach in which the higher energy states are missing and in practice a free theory is assumed above the energy determined by the BD cutoff Λ. We compared the effective interactions obtained in the explicit and implicit renormalization approaches and analyzed to what extent in terms of the BD cutoff Λ the two approaches overlap. Here we restrict the analysis to the case of the $^1S_0$ channel NN interaction. We also discuss the results of a preliminary study on the role played by the one-pion exchange (OPE) interaction which is carried out by implementing the BD-SRG evolution of the δ-shell plus OPE representation for the NN interaction described in Ref. [22].

2. Toy-model separable gaussian potential

In the applications of the SRG method to nuclear physics, realistic potentials which fit NN scattering data up to the pion-production threshold ($\sqrt{m_\pi M_N} \sim 400$ MeV) are usually taken as the initial NN *bare* interaction. Due to the short-range repulsive core, such potentials exhibit a long high-momentum tail which complicates the numerical convergence when solving the SRG flow-equations. Therefore, for illustration purposes, we will consider here as the NN *bare* interaction a simple separable gaussian potential in the $^1S_0$ channel, given by

$$V(p, p') = C \; g_L(p)g_L(p') = C \; \exp\left[-\left(p^2 + p'^2\right)/L^2\right] \; . \tag{1}$$
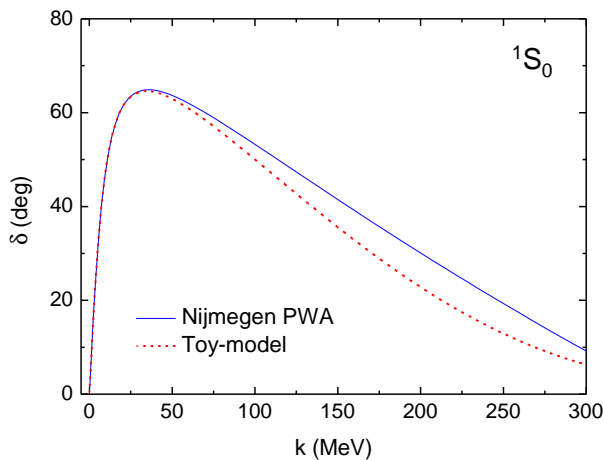
Figure 1. Phase-shifts for the toy-model potential in the $^1S_0$ channel compared to the results obtained from the Nijmegen PWA [13].

The parameters C and L are determined from the solution of the Lippmann-Schwinger (LS) equation for the on-shell reactance matrix K by fitting the experimental values of the Effective Range Expansion (ERE) parameters. Namely, we solve the partial-wave LS equation for the K-matrix,

$$K(p, p'; E) = V(p, p') + \frac{2}{\pi} \mathcal{P} \int_0^\infty dq \, q^2 \, \frac{V(p, q)}{E - q^2} \, K(q, p'; E) \,, \qquad (2)$$

where E is the scattering energy, and match the resulting on-shell K-matrix to the ERE expansion,

$$K^{-1}(k, k; k^2) = -\left[-\frac{1}{a_0} + \frac{1}{2} \, r_e \, k^2 + \mathcal{O}(k^4) \right] = -k \, \cot \delta(k) \,, \qquad (3)$$

where $k = \sqrt{E}$ is the on-shell momentum and $\delta(k)$ stands for the phase-shifts. Adjusting the parameters of the toy model potential in the $^1S_0$ channels to fit the ERE parameters to second order in the on-shell momentum k, i.e. the scattering length $a_0 = -23.74$ fm and the effective range $r_e = 2.77$ fm we obtain $C = -1.915884$ fm and $(1/L^2) = 0.691269$ fm^2.

In the case of the toy-model separable potential, given by Eq. (1), it is straightforward to evaluate the phase-shifts $\delta(k)$ from the solution of the partial-wave LS equation for the K-matrix using the *ansatz*

$$K(p, p'; k^2) = g_L(p) \, \tilde{K}(k) \, g_L(p') \,, \qquad (4)$$

where $\tilde{K}(k)$ is called the reduced on-shell K-matrix. This leads to the relation

$$k \cot \delta(k) = -\frac{1}{V(k, k)} \left[1 - \frac{2}{\pi} \mathcal{P} \int_0^\infty dq \, q^2 \frac{1}{k^2 - q^2} V(q, q) \right] \,. \qquad (5)$$

The phase-shifts for the toy-model potential in the $^1S_0$ channel evaluated from this equation are shown in Fig. 1, compared to the results obtained from the Nijmegen partial-wave analysis (PWA) [13]. As one can see, despite its simplicity, our toy model for the NN interaction provides a reasonable qualitative description of the $^1S_0$ phase-shifts.

3. Explicit renormalization: BD-SRG evolution

The similarity renormalization group (SRG) approach, developed by Glazek and Wilson [23] and independently by Wegner [24], is a renormalization method based on a series of continuous unitary transformations that evolve hamiltonians with a cutoff on energy differences, driving the original hamiltonian towards a band-diagonal form. Here we employ the formulation for the SRG developed by Wegner, which is based on a non-perturbative flow-equation that governs the unitary evolution of a hamiltonian $H = T_{\rm rel} + V$ with a flow parameter s that ranges from zero to infinity. Namely, assuming that $T_{\rm rel}$ is independent of s, we have

$$\frac{dH_s}{ds} = \frac{dV_s}{ds} = [\eta_s, H_s] \,, \tag{6}$$

where η_s is an anti-hermitian operator. The flow parameter s has dimensions of $[\text{energy}]^{-2}$ and in terms of the SRG cutoff λ with dimension of momentum is given by the relation $s = \lambda^{-4}$. The flow equation is to be solved with the boundary condition $H_s|_{s\to 0} \equiv H_0$, where $H_0 (\equiv H_{\lambda \to \infty})$ is the hamiltonian corresponding to the initial *bare* interaction.

The anti-hermitian operator η_s is usually chosen as $\eta_s = [G_s, H_s]$, where G_s is a hermitian operator which we call the SRG generator since it defines η_s and so the flow of the hamiltonian. Here, we take the block-diagonal (BD) SRG generator [21], given by

$$G_s = H_s^{\rm BD} \equiv \begin{pmatrix} PH_sP & 0 \\ 0 & QH_sQ \end{pmatrix} \,, \tag{7}$$

where P and $Q = 1 - P$ are projection operators. In a partial-wave momentum-space basis, the projection operators are determined in terms of the BD cutoff Λ that divides the momentum space into a low-momentum P-space ($p < \Lambda$) and a high-momentum Q-space ($p > \Lambda$). Here we define the projection operators just as step functions, $P \equiv \theta(\Lambda - p)$; $Q \equiv \theta(p - \Lambda)$.

Thus, the flow-equation with the BD-SRG generator can be written in matrix-form as

$$\begin{pmatrix} \frac{d}{ds}[PV_sP] & \frac{d}{ds}[PV_sQ] \\ \frac{d}{ds}[QV_sP] & \frac{d}{ds}[QV_sQ] \end{pmatrix} = \begin{pmatrix} P\eta_sQH_sP - PH_sQ\eta_sP & P\eta_sQH_sQ - PH_sP\eta_sQ \\ Q\eta_sPH_sP - QH_sQ\eta_sP & Q\eta_sPH_sQ - QH_sP\eta_sQ \end{pmatrix} \,. \tag{8}$$

This equation has to be solved numerically on a finite momentum grid with N points p_n and weights w_n ($n = 1, \ldots N$) by implementing a high-momentum ultraviolet cutoff $P_{\max}$ and an infrared momentum cutoff $P_{\min}$. The discretization of the momentum space on a grid with N points leads to a system of $4N^2$ non-linear first-order coupled differential equations. By choosing the BD-SRG generator $G_s = H_s^{\rm BD}$, the matrix-elements inside the off-diagonal blocks PV_sQ and QV_sP are suppressed as the flow parameter s increases (or as the similarity cutoff λ decreases), such that the hamiltonian is driven to a block-diagonal form. In the infrared limit $s \to \infty$ ($\lambda \to 0$) the P-space and the Q-space become completely decoupled, i.e.

$$\lim_{s\to 0} \begin{pmatrix} PV_sP & PV_sQ \\ QV_sP & QV_sQ \end{pmatrix} = \begin{pmatrix} PV_{\rm low\,k}P & 0 \\ 0 & QV_{\rm high\,k}Q \end{pmatrix} \,. \tag{9}$$

Thus, while unitarity implies that the phase-shifts evaluated from the solution of the LS equation remain invariant along the SRG evolution, i.e. $\delta_\lambda(p) = \delta(p)$ for any λ, one has

$$\lim_{\lambda \to 0} \delta_\lambda(p) = \delta_{\rm low\,k}(p) + \delta_{\rm high\,k}(p) \,, \tag{10}$$

where $\delta_{\rm low\,k}(p) = \delta(p)\theta(\Lambda - p)$ and $\delta_{\rm high\,k}(p) = \delta(p)\theta(p - \Lambda)$ are the phase-shifts of the $V_{\rm low\,k}$ and $V_{\rm high\,k}$ potentials respectively.

4. Implicit renormalization

Implicit renormalization can be defined in simple way by looking for an effective NN interaction regulated by a sharp or smooth momentum cutoff Λ which reproduces NN scattering data up to a given center-of-mass (CM) momentum $k \leq \Lambda$. The requirement that observables should be cutoff independent determines the implicit Λ-dependence of the effective interaction.

At low cutoffs Λ, we may approximate the toy-model potential by an effective field theory (EFT) with only contact interactions regulated by a smooth exponential momentum cutoff,

$$V_\Lambda(p, p') = \exp[-(p/\Lambda)^{2n})] \left[C_0 + C_2(p^2 + p'^2) + \ldots \right] \exp[-(p'/\Lambda)^{2n}], \qquad (11)$$

where $C_0, C_2, \ldots$ are Λ-dependent coefficients to be determined through a renormalization procedure and $n = 1, 2, \ldots$ defines the sharpness of the cutoff regulating function.

The running of the coefficients C_i with the cutoff Λ is determined from the solution of the LS equation for the on-shell K-matrix by fitting the experimental values of the ERE parameters. For the contact theory potential at next-to-leading order (NLO) the coefficients $C_0^{(2)}$ and $C_2^{(2)}$ are fixed at a given cutoff Λ by fitting the scattering length a_0 and the effective range r_e. One should note that, as a consequence of the Wigner causality bound, there is a maximum value Λ_{WB} for the cutoff Λ above which we cannot fix the NLO potential coefficients by fitting the experimental values of both a_0 and r_e while keeping the renormalized potential hermitian [25].

5. Comparison between the explicit and the implicit renormalization approaches

We solve the BD-SRG flow equation for the toy-model potential in the $^1S_0$ channel on a gaussian grid with $N = 50$ points and $P_{\max} = 5$ fm^{-1}, using an adaptative variable-step fifth-order Runge-Kutta algorithm. Then, we compare the running of the coefficients $C_0^{(2)}$ and $C_2^{(2)}$ with the cutoff Λ in the effective NLO contact theory potential on the same grid to the running of the corresponding coefficients $\tilde{C}_0^{(2)}$ and $\tilde{C}_2^{(2)}$ with the BD cutoff ($\equiv \Lambda$) extracted from a polynomial fit of the BD-SRG evolved toy-model potential,

$$V_{\lambda,\Lambda}(p, p') = \tilde{C}_0^{(2)} + \tilde{C}_2^{(2)} \, (p^2 + p'^2) + \cdots . \qquad (12)$$

The parameters C and L in the initial toy-model potential and the coefficients $C_0^{(2)}$ and $C_2^{(2)}$ in the NLO contact theory potential are determined from the numerical solution of the LS equation for the K-matrix by fitting the experimental values of a_0 and r_e. The coefficients $\tilde{C}_0^{(2)}$ and $\tilde{C}_2^{(2)}$ are determined by fitting the diagonal matrix-elements of the BD-SRG evolved toy-model potential for the lowest grid momenta with the polynomial form.

In Fig. 2 we show the density plots for the BD-SRG evolution of the toy-model potential in the $^1S_0$ channel for a BD cutoff $\Lambda = 0.5$ fm^{-1} [18]. As expected, the P-space and the Q-space become decoupled as the SRG cutoff λ decreases towards the infrared limit $\lambda \to 0$. In Fig. 3 we show the results for the coefficients $\tilde{C}_0^{(2)}$ and $\Lambda^2 \tilde{C}_2^{(2)}$ extracted from the BD-SRG evolved toy-model potential in the $^1S_0$ channel compared to the corresponding coefficients $C_0^{(2)}$ and $\Lambda^2 C_2^{(2)}$ obtained for the NLO contact theory potential regulated by a smooth exponential momentum cutoff with a sharpness parameter $n = 16$. As one can see, there is a remarkably good agreement between the coefficients extracted from the BD-SRG evolved potential and those obtained for the NLO contact theory potential as the SRG cutoff λ decreases, which can be traced to the decoupling between the P-space and the Q-space. Thus, in the infrared limit $\lambda \to 0$ we expect to achieve a high degree of agreement between the effective interactions obtained in the explicit and the implicit renormalization approaches for BD cutoffs Λ up to Λ_{WB} determined by the Wigner causality bound for the NLO contact theory potential. Indeed, for the lowest SRG cutoff considered in the calculations, $\lambda = 0.1$ fm^{-1}, the overlap between the two approaches is verified within a range of BD cutoffs Λ from 0.5 fm^{-1} to 1.5 fm^{-1}.
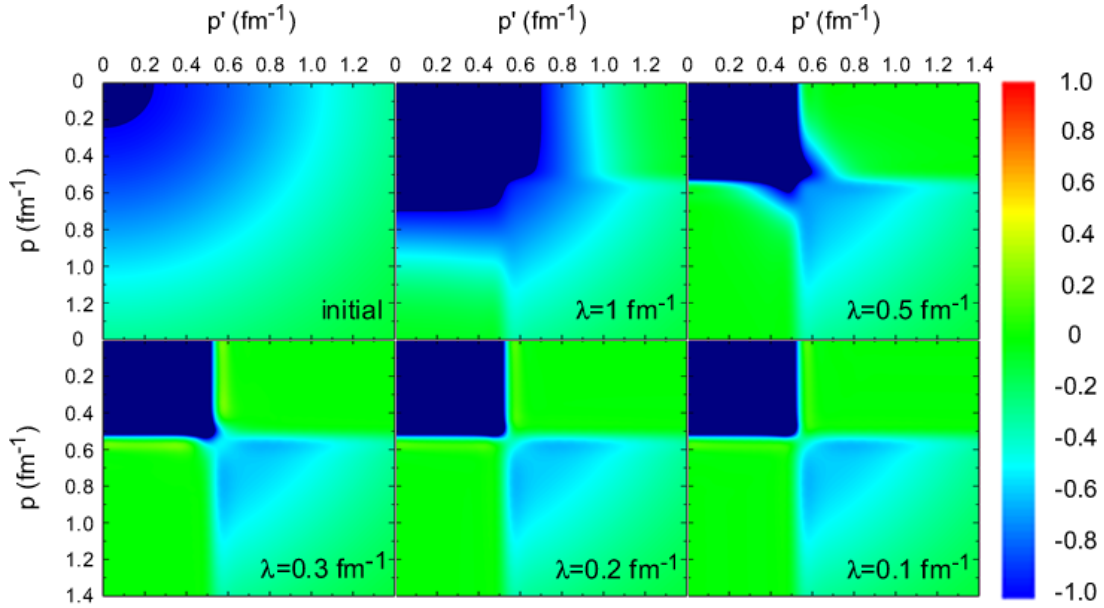
Figure 2. Density plots for the BD-SRG evolution of the toy-model potential in the $^1S_0$ channel for a BD cutoff $\Lambda = 0.5$ fm^{-1} ($N = 50$ points and $P_{\max} = 5$ fm^{-1}) [18].
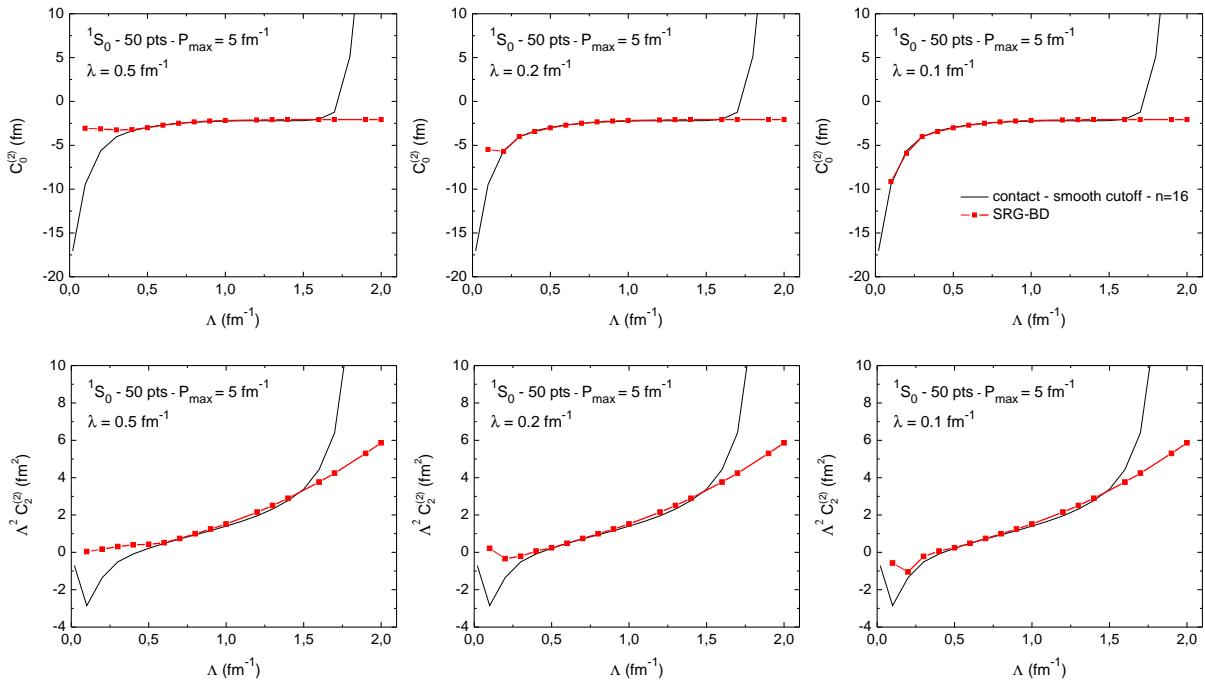

Figure 3. Coefficients $\tilde{C}_0^{(2)}$ and $\Lambda^2 \tilde{C}_2^{(2)}$ extracted from the BD-SRG evolved toy-model potential in the $^1S_0$ channel compared to the corresponding coefficients $C_0^{(2)}$ and $\Lambda^2 C_2^{(2)}$ for the *NLO* contact theory potential regulated by a smooth exponential momentum cutoff with $n = 16$.

6. Role of the one-pion exchange

As we have pointed out, the agreement between the effective interactions obtained in the explicit and implicit renormalization approaches over a wide range of relatively low cutoff scales Λ is due to the decoupling between the low-momentum P-space and the high-momentum Q-space. This motivates an analysis of the role played by the OPE interaction in the implicit approach.

We consider the δ-shell (DS) plus OPE representation for the NN interaction described in Ref. [22], built with basis on a PWA of about 8000 pp and np data. According to this analysis, OPE is the only needed contribution for $r > 3$ fm such that the NN interaction can be split as

$$V = V(r \leq 3 \text{ fm}) + V(1\pi, r \geq 3 \text{ fm}) \,, \tag{13}$$

where $V(r \leq 3 \text{ fm})$ corresponds to the short- and intermediate-range interactions parametrized through the δ-shells and $V(1\pi, r \geq 3 \text{ fm})$ corresponds to the long-range OPE interaction. In the top-panels of Fig. 4 we show the diagonal and fully off-diagonal matrix-elements of the DS + OPE potential in the $^1S_0$ channel, together with the corresponding contributions from $V(r \leq 3 \text{ fm})$ and $V(1\pi, r \geq 3 \text{ fm})$. As one can see, $V(1\pi, r \geq 3 \text{ fm}) \ll V(r \leq 3 \text{ fm})$ and hence it might be possible to implement a perturbative expansion of the BD-SRG evolved DS + OPE potential in which only the $V(r \leq 3 \text{ fm})$ piece is evolved and the corrections from the evolved OPE are included order by order, i.e.

$$V_{\lambda,\Lambda} \equiv V_{\lambda,\Lambda}(r \leq 3 \text{ fm}) + V(1\pi, r \geq 3 \text{ fm}) + \mathcal{O}\left[V_{\lambda,\Lambda}^2(1\pi, r \geq 3 \text{ fm})\right] \,. \tag{14}$$

In the bottom panels of Fig. 4 we show the diagonal and fully off-diagonal matrix-elements of the difference between the full DS + OPE potential in the $^1S_0$ channel evolved with the BD-SRG up to $\lambda = 1$ fm^{-1} and the zeroth-order perturbative approximation for several values of the BD cutoff Λ. We get that the corrections from the BD-SRG evolved OPE piece are indeed small, namely $\mathcal{O}[V_{\lambda,\Lambda}^2(1\pi, r \geq 3 \text{ fm})] \leq 10^{-2}$ fm for 0.5 fm$^{-1} \leq \Lambda \leq 3.0$ fm^{-1}. This result suggests that the contribution from the BD-SRG evolved OPE interaction may be treated perturbatively.

7. Summary and Outlook

We have presented a summary of our previous works on the application of the block-diagonal similarity renormalization group (BD-SRG) to the NN interaction, whose main purpose was to investigate the complementarity between the implicit and the explicit renormalization approaches in nuclear physics. In order to simplify the analysis and reduce the computational effort, we have considered a separable gaussian potential toy-model for the NN interaction in S-wave channels. Here we have focused on the analysis of the NN system in the $^1S_0$ channel.

By comparing the NN effective interactions obtained both in the explicit and the implicit renormalization schemes, we verify that the complementarity between these two approaches holds for a wide range of cutoff scales Λ. This suggests that the bulk of the effective NN interaction and its scale dependence can be extracted directly from low-energy NN data. We have also presented a preliminary analysis of the role played by the OPE interaction, based on a perturbative expansion of the BD-SRG evolved $^1S_0$ channel NN potential in a δ-shell plus OPE representation. As we have shown, the contribution from the OPE interaction remains small after the BD-SRG evolution, suggesting that it may be treated perturbatively in calculations of light nuclei structure. In a forthcoming publication we will present a detailed study on this issue, including also an analysis of the relevance of the two-pion exchange (TPE) interaction.
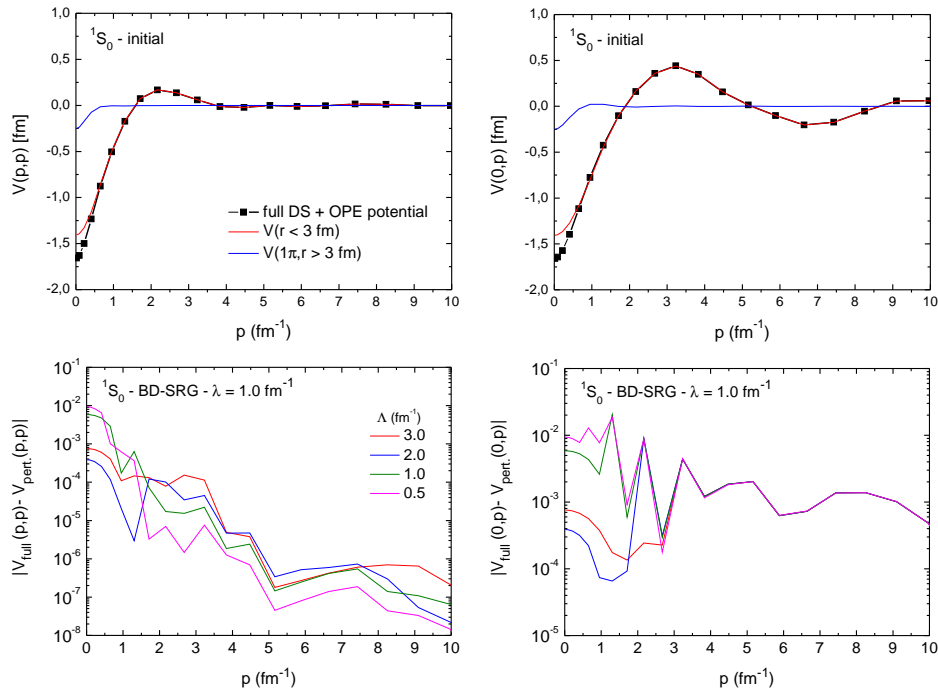
Figure 4. Top-panels: diagonal and fully off-diagonal matrix-elements of the DS + OPE potential in the $^1S_0$ channel, together with the corresponding contributions from $V(r \leq 3 \text{ fm})$ and $V(1\pi, r \geq 3 \text{ fm})$; Bottom panels: diagonal and fully off-diagonal matrix-elements of the difference between the full DS + OPE potential evolved with the BD-SRG up to $\lambda = 1 \text{ fm}^{-1}$ and the zeroth-order perturbative approximation for several values of the BD cutoff Λ.

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