Variational Calculations using Low-Momentum Potentials with Smooth Cutoffs

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Abstract

Recent variational calculations of the deuteron and the triton illustrate that simple wave function ansätze become more effective after evolving the nucleon-nucleon potential to lower momentum (“$V_{\text{low } k}$”). However, wave function artifacts from the use of sharp cutoffs in relative momentum decrease effectiveness for small cutoffs ($< 2 \text{fm}^{-1}$) and slow down convergence in harmonic oscillator bases. These sharp cutoff artifacts are eliminated when $V_{\text{low } k}$ is generated using a sufficiently smooth cutoff regulator.

1 Introduction

Variational calculations for nuclei are complicated by the strong short-range repulsion and tensor forces of conventional nucleon-nucleon potentials, which necessitate highly correlated trial wave functions. However, the nonperturbative nature of conventional inter-nucleon interactions is strongly scale or resolution dependent and can be radically modified by using the renormalization group (RG) to lower the momentum cutoff of the two-nucleon potential [1]. A particular consequence is that the short-range correlations in few- and many-body wave functions are significantly reduced at lower resolutions [1]. This has the practical implication that variational calculations should be more effective at lower cutoffs using simple wave function ansätze. A recent study using low-momentum potentials (generically called “$V_{\text{low } k}$”) supports this claim [2]. This conclusion is also consistent with the results of Viviani et al. [3],

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who showed that variational calculations of 3– and 4–body nuclei using hyperspherical harmonics converge faster for potentials with greater nonlocality, which reduces short-range correlations.

The optimistic conclusions regarding the use of $V_{\text{low}k}$ in variational calculations are clouded by some problems associated with the sharp momentum cutoff, which are of concern for some practical applications. In particular, one would expect that for very-low-energy observables such as the deuteron or triton binding energies, there should be improved variational estimates down to very low cutoffs (e.g., comparable to the “binding momentum”), and rapid convergence with basis size. However, what was observed in Ref. [2] was improvement down to moderate cutoffs of $2\text{ fm}^{-1}$ followed by a degradation of the variational estimates at smaller cutoffs. Further, for a wide range of cutoffs the convergence of the triton binding energy with the size of a harmonic oscillator basis was exceedingly slow once the energy prediction was at the 100\,keV level. Both of these problems were attributed to the use of a sharp cutoff on the relative momentum. In this letter, we revisit the variational calculations in Ref. [2] to demonstrate that these limitations can be eliminated by constructing $V_{\text{low}k}$ potentials using a smooth regulator. There are many new issues to consider with such a regulator, but we defer most of the further discussion to a more complete and wide-ranging investigation [4].

2 $V_{\text{low}k}$ with a Smooth Regulator

The construction of $V_{\text{low}k}$ with a sharp cutoff is documented in Refs. [5,6], where it is shown that either RG equations or Lee-Suzuki transformations can be used. The latter approach relies heavily on the introduction of orthogonal low- and high-energy subspaces with projection operators $P$ and $Q$, such that $P + Q = 1$ and $PQ = QP = 0$. In momentum space for the two-nucleon system, the last condition mandates a sharp cutoff $\Lambda$ in relative momentum, so that $P$-space integrals run from 0 to $\Lambda$ while $Q$-space integrals run from $\Lambda$ to $\infty$ (or to a large bare cutoff). But while replacing a sharp cutoff with a regulator that smoothly cuts off the relative momentum seems incompatible with methods requiring $PQ = 0$, it is not a conceptual problem for the more general RG approach [5]. Details will be presented in Ref. [4]; here we simply summarize a three-step procedure applied in the present calculations.

Smooth cutoff regulators will be applied in each partial wave as simple functions of the relative momentum. It is convenient and efficient for numerical calculations to define the smoothly regulated energy-independent potential $V_{\text{low}k}$ and the corresponding $T_{\text{low}k}$ matrix in terms of a reduced potential $v$
and a reduced $T$ matrix $t$ as

$$V_{\text{low}k}(k', k) = f(k')v(k', k)f(k),$$

(1)

and

$$T_{\text{low}k}(k', k; k^2) = f(k')t(k', k; k^2)f(k),$$

(2)

where $f(k)$ is a smooth cutoff function. Here we adopt for $f(k)$ the exponential form used in chiral EFT potentials at N$^3$LO order [7],

$$f(k) = e^{-k^2/\Lambda^2}.$$  

(3)

We use $n = 4$ throughout this work. The reduced $t$ matrix obeys a Lipmann-Schwinger equation with loop integrals smoothly cut off by the internal factors of $f(p)$ [5],

$$t(k', k; k^2) = v(k', k) + \frac{2}{\pi} \int_0^\infty p^2 dp \frac{v(k', p)f^2(p)t(p, k; k^2)}{k^2 - p^2}.$$  

(4)

Note that the cutoff is on the loop momentum but not on external momenta. Principal value integrals are implicit throughout.

In the energy-independent RG approach, an RG equation for the reduced interaction $v(k', k)$ is derived by demanding that $\frac{d}{d\Lambda} t(k', k; k^2) = 0$. 1 Using the large-cutoff initial condition $v(k', k) = V_{NN}(k', k)$, the resulting set of coupled differential equations can be numerically integrated to evolve the interaction to lower cutoffs. The resulting $V_{\text{low}k}$ preserves the original on-shell $T$ matrix up to factors of the smooth regulator,

$$T_{\text{low}k}(k; k^2) = f^2(k)T_{NN}(k; k^2),$$

(5)

which implies that low-energy phase shifts are preserved for on-shell momenta away from the transition region near the cutoff where the regulator function rapidly decreases to zero. While the energy-independent RG approach provides a direct path to construct the smooth cutoff version of $V_{\text{low}k}$, it is not the most convenient or numerically robust method [4].

In this work, we prefer to use a much simpler energy-dependent RG equation to evolve the bare potential $V_{NN}$ to a lower cutoff. The energy-dependent RG equation is obtained by requiring invariance of the full off-shell $T$ matrix, $\frac{d}{d\Lambda} t(k', k; E) = 0$, which can be formally integrated [4] to recover the Bloch-Horowitz equation with a smooth cutoff:

$$v(k', k; E) = V_{NN}(k', k) + \frac{2}{\pi} \int_0^\infty p^2 dp \left( 1 - f^2(p) \right) \frac{V_{NN}(k', p)v(p, k; E)}{E - p^2}.$$  

(6)

1 This RG equation generates a non-hermitian interaction. Hermiticity can be restored by using a symmetrized form of the RG equation [4]. The resulting interaction preserves the on-shell $T$ matrix, but no longer preserves the half-offshell $T$ matrix.
The resulting integral equation for $v(k', k; E)$ is much more efficient for numerical calculations than the original set of coupled differential equations.

The second step is to trade the energy dependence for momentum dependence by defining an energy-independent (but non-hermitian) $V_{\text{low}}(k', k)$ that gives the same half-on-shell $T$ matrix and wave functions as the energy-dependent interaction $V_{\text{eff}}(k', k; E) = f(k')v(k', k; E)f(k)$,

$$
\langle k' | V_{\text{eff}}(p^2) | \Psi_p \rangle = \langle k' | V_{\text{low}} | \Psi_p \rangle .
$$

The $\Psi_p$ are the self-consistent wave functions of the energy-dependent low-momentum Hamiltonian $H_{\text{eff}}(p^2)$. Using the completeness of these wave functions, one obtains a simple expression for the non-hermitian $V_{\text{low}}$,

$$
V_{\text{low}}(k', k) = \left( \frac{2}{\pi} \right)^2 \int_0^\infty p^2 dp \int_0^\infty k'^2 dk'' V_{\text{eff}}(k', k''; p^2) \Psi_p(k'') \bar{\Psi}_p^*(k) ,
$$

where $\bar{\Psi}_p^*$ is the biorthogonal complement wave function. Note that the integral over the continuous scattering states will include a summation over discrete bound states, when present.

The final step is to apply a Gram-Schmidt procedure to hermitize the potential, as prescribed in Ref. [8]. The end result is a hermitian, energy-independent $V_{\text{low}}$ with a smooth cutoff regulator that preserves the low energy on-shell $T$ matrix up to factors of the regulator as in Eq. (5). In addition, the complete set of wave functions obtained from diagonalizing $H_{\text{low}}$ can be used to consistently evolve general operators beyond the Hamiltonian with the smooth cutoff. Thus, the present approach may be viewed as a generalization of conventional effective interaction methods such as Lee-Suzuki transformations to smooth cutoffs. Further details concerning the present approach as well as the energy-independent RG method will be provided in Ref. [4].

As in Ref. [2], we will show results starting from the Argonne $v_{18}$ potential [10] as $V_{NN}$, since it has been used in almost all modern calculations of light nuclei. However, as with the sharp cutoff $V_{\text{low}}$ calculations, the pattern of results for the full cutoff range shown here does not vary significantly with different initial potentials. When using the sharp cutoff $V_{\text{low}}$, two-body bound-state properties and phaseshifts are preserved by construction for external relative momenta right up to the cutoff. (Note that three- and many-body observables require the consistent addition of a three-body force to remove cutoff dependence [9].) The use of a smooth regulator, however, distorts the phaseshifts near the cutoff according to Eq. (5) to a degree that depends on the type of regulator function [4]. These distortions are not important for the low-energy observables discussed here, but will need further assessment for future applications.
Since the final $V_{\text{low } k}$ is energy independent and hermitian, variational calculations proceed as described in ordinary quantum mechanics texts (e.g., without special normalizations as needed for energy-dependent potentials). That is, given a trial wave function $\psi_{\text{trial}}$, our variational estimate for the ground state energy at cutoff $\Lambda$ is:

$$E_{\text{var}}(\Lambda) = \frac{\langle \psi_{\text{trial}} | T + V_{\text{low } k}(\Lambda) | \psi_{\text{trial}} \rangle}{\langle \psi_{\text{trial}} | \psi_{\text{trial}} \rangle} ,$$

which we minimize with respect to the parameters in $\psi_{\text{trial}}$. Alternatively, we get a variational estimate by diagonalizing $T + V_{\text{low } k}(\Lambda)$ in a truncated basis, where the trial wavefunction is a linear combination of the basis functions.

### 3 Variational Results for the Deuteron and Triton

Here we retrace the calculations of Ref. [2], starting with a study of the deuteron binding energy. As noted there, for weakly bound states we expect that a simple, generic ansatz should work increasingly well as the cutoff is lowered. Two such ansätze were considered. In the first one [11], the (un-normalized) $^3S_1$ and $^3D_1$ trial functions for the deuteron are (following the conventions of Ref. [12])

$$\psi_0(k) = \frac{1}{(k^2 + \gamma^2)(k^2 + \mu^2)} , \quad \psi_2(k) = \frac{a k^2}{(k^2 + \gamma^2)(k^2 + \nu^2)} ,$$

where $\gamma, \mu, \nu, \text{ and } a$ are variational parameters. The underlying physics implies that $\mu$ and $\nu$ should be roughly the inverse range of the interaction and $\gamma$ should be close to $(-M_N E_d)^{1/2}$, where $M_N$ is the mean neutron-proton mass and $E_d \approx -2.2246 \text{ MeV}$ is the deuteron binding energy. The regulator in $V_{\text{low } k}$ implies that the corresponding exact deuteron wave function does not contain high-momentum components. Therefore, the two-body trial wave functions are multiplied by the same regulator $f(k)$ for the relative momentum.

We also adapted the form used for a high-accuracy representation of the deuteron wave function in Ref. [12], for which

$$\psi_0(k) = f(k) \sum_{j=1}^{j_{\text{max}}} \frac{C_j}{k^2 + m_j^2} , \quad \psi_2(k) = f(k) \sum_{j=1}^{j_{\text{max}}} \frac{D_j}{k^2 + m_j^2} ,$$

where the $m_j$ are fixed in a geometric progression:

$$m_j = (-M_N E_d)^{1/2} + (j - 1)m_0 , \quad \text{with } m_0 = 0.9 \text{ fm}^{-1} ,$$

by treating the $C_j$ and $D_j$ coefficients as variational parameters for a given value of $j_{\text{max}}$. (The very accurate parameterization of the deuteron wave func-
\begin{equation} \Lambda^{(m)} \end{equation}

\begin{equation} E_{d}^{\text{var}} - E_{d} \end{equation}

Fig. 1. Deviation from $E_{d}$ of the best variational energy as a function of cutoff $\Lambda$ for the wave function ansätze of Eqs. (10) and (11) with different numbers of terms. Smooth cutoff $V_{\text{low},k}$ results are given by the open symbols.

The best variational energy for Eq. (10) as a function of a sharp cutoff is shown as the filled squares in Fig. 1. These estimates are not even bound for cutoffs above $\Lambda \approx 5 \text{ fm}^{-1}$ (which includes the bare Argonne $v_{18}$ potential) but rapidly improve as the cutoff is lowered further, reaching a minimum deviation of less than 3 keV around $\Lambda \approx 1.5 \text{ fm}^{-1}$. Similar results are found for the ansatz of Eq. (11) with $j_{\text{max}} = 3$ (solid diamonds) and $j_{\text{max}} = 4$ (solid circles). As expected, lowering the sharp cutoff dramatically improves the effectiveness of the simple wave function ansätze, but the results unexpectedly worsen for cutoffs that are significantly larger than the naive limiting value set by the “binding momentum” of the deuteron, $\Lambda_{d} \approx 0.25 \text{ fm}^{-1}$.

The variational estimates for the smooth cutoff of Eq. (3) are shown in Fig. 1 as unfilled symbols for the corresponding ansätze. For the ansatz of Eq. (10), the smooth cutoff results are inferior at intermediate cutoffs but continue to improve monotonically at smaller cutoffs. For the other ansatz, the smooth-cutoff results are superior throughout and improve until reaching agreement with the exact result at the eV level. This is in accord with intuition for such a low-energy bound state, and it emphasizes that one works much too hard in calculating low-energy observables using conventional potentials that contain
The reduced effectiveness of simple ansätze for the deuteron when using sharp cutoffs below 2 fm\(^{-1}\) can be understood by looking at the corresponding wave functions in momentum space. In Fig. 2, we show the exact deuteron wave functions in momentum space for both the smooth and sharp cutoffs at \(\Lambda = 1.6\) fm\(^{-1}\) and 2 fm\(^{-1}\). The \(V_{\text{low} k}\) wave functions remove the short-range/high-momentum behavior (e.g., the node just above 2 fm\(^{-1}\) [13]) that is increasingly resolved at higher cutoffs, requiring finer and finer cancellations in the variational integrals and a more correlated wave function. At \(\Lambda = 2\) fm\(^{-1}\), the sharp wave function is well behaved and an ansatz cutoff at the same momentum is adequate for a momentum-space variational calculation. (Even here, the abrupt cutoff creates problems in coordinate-space calculations, particular for the \(^3D_1\) component of the wave function.) But by \(\Lambda = 1.6\) fm\(^{-1}\), one clearly sees a complicated endpoint behavior that will not be reproduced in simple variational trial functions. In contrast, the smooth regulator potential and corresponding wave functions do not have these artifacts.

The extension from the deuteron to the triton in Ref. [2] was kept simple by using a truncated harmonic oscillator basis for a variational calculation with the two-body interaction only, which we repeat here for the smoothly regulated \(V_{\text{low} k}\) potentials. The antisymmetric three-nucleon basis is generated from the
Fig. 3. Convergence of the binding energy of the triton from a direct diagonalization of the Hamiltonian in a harmonic-oscillator basis with fixed oscillator parameter $b_{\text{osc}} = 1.5 \text{ fm}$. Results for two cutoffs are shown. In each case the filled symbols are for a sharp cutoff and the unfilled symbols are for a smooth cutoff.

Jacobi coordinate oscillator states [14]

$$|(nlsjt; \mathcal{N}\mathcal{L}_{\frac{1}{2}}\mathcal{J}_{\frac{1}{2}})JT\rangle,$$

(13)

where $(nlsjt)$ and $(\mathcal{N}\mathcal{L}_{\frac{1}{2}}\mathcal{J}_{\frac{1}{2}})$ are the quantum numbers corresponding to the two relative Jacobi coordinates [e.g., $k = \frac{1}{2}(p_1 - p_2)$ and $q = \frac{5}{3}(p_3 - \frac{1}{2}(p_1 + p_2))$], and the basis is truncated according to the total number of oscillator quanta $N = (2n + l + 2\mathcal{N} + \mathcal{L}) \leq N_{\text{max}}$. Diagonalizing the intrinsic Hamiltonian in the truncated basis and minimizing with respect to the oscillator length parameter $b$ provides a variational estimate to the true ground-state energy.

The same pattern of the variational estimates for sharp cutoffs seen for the deuteron, namely improvement to a minimum followed by worsening estimates for very low $\Lambda$, was observed for the triton in Ref. [2]. However, an additional problem of convergence with the size of the harmonic oscillator basis, which is of greater practical importance, was seen as well over a wide range of cutoffs. For cutoffs around $2 \text{ fm}^{-1}$, energies within about 200 keV of the accurate result from Fadeev calculations are reached with relatively small basis size, but then further convergence as the basis is increased is extremely slow (see the filled symbols in Fig. 3). In fact, extremely slow convergence beyond the 50 keV level is found for a wide range of cutoffs. One expects convergence at the keV
The poor convergence of the sharp cutoff $V_{low k}$ in an oscillator basis is analogous to “Gibbs overshoot” phenomena found in Fourier series expansions of discontinuous functions. This connection is supported by noting the rapid convergence of the energy with the smooth cutoff $V_{low k}$ (e.g., the unfilled squares for $\Lambda = 2.0 \text{ fm}^{-1}$ in Fig. 3 are within 2 keV at $N_{\text{max}} = 20$ and within 1 keV at $N_{\text{max}} = 30$ of the converged result). Similar dramatically improved convergence using the smooth cutoff $V_{low k}$ is also found at other cutoffs (e.g., the unfilled circles in Fig. 3).

Fadeev results with smooth cutoffs are not yet available to verify that they agree with the converged energies obtained here. However, we can look back at deuteron calculations using a harmonic oscillator basis to anticipate what we will find. Figure 4 shows the deviation of the variational estimate from the exact deuteron binding energy for a harmonic oscillator basis, comparing the two types of regulator. Each point was optimized with respect to the oscillator parameter in a basis of fixed size $N_{\text{max}} = 40$. As found for the other ansätze, the smooth cutoff improves steadily with decreasing $\Lambda$. We expect similar behavior for the triton.\(^2\)

\(^2\) We do not expect the addition of consistent three-body forces, which have been
4 Conclusions

In summary, use of a smooth cutoff regulator preserves the improvement with lower cutoff and remedies the technical problems noted in Ref. [2] for variational calculations of the deuteron and triton with low-momentum potentials. While the deuteron and triton are not stringent tests for heavier nuclei, these results coupled with the rapid convergence of the particle-particle channel observed in nuclear matter [1] imply that low-momentum potentials will be much more effective for few-body and many-body variational calculations than any conventional large-cutoff potential. Investigations of the effectiveness of running a smooth cutoff lower for chiral EFT potentials, which are themselves low-momentum potentials compared to conventional potential models, will be explored elsewhere along with many other issues [4].

To take advantage of these observations, the variational calculations described recently in Ref. [3], which show the advantages of nonlocal interactions, should be particularly well suited. Based on our results here, we anticipate even more efficient variational results for low-momentum interactions with smooth cutoffs, with the added advantage of being able to vary the cutoff as a tool to optimize and probe the quality of the solution. Furthermore, we can avoid the problem of constructing consistent, model-independent operators for conventional potentials by concurrently evolving to low momentum the potential and operators from chiral EFT.

Since Hartree-Fock becomes a reasonable starting point for nuclear many-body calculations [1], the large arsenal of techniques developed for the Coulomb many-body problem becomes available and should be explored as well. In addition, the development of the smooth cutoff $V_{low\,k}$ allows one to unambiguously perform a density matrix expansion starting from low-momentum interactions to gain insight into the microscopic foundation of the nuclear energy density functional, as the required coordinate space quantities are now well-defined with the smooth cutoff [15].

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shown to become more perturbative with lower cutoffs [9,1], to alter this assessment.
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