Accelerating Convergence by Change of Basis for No-Core Configuration Interaction Calculations

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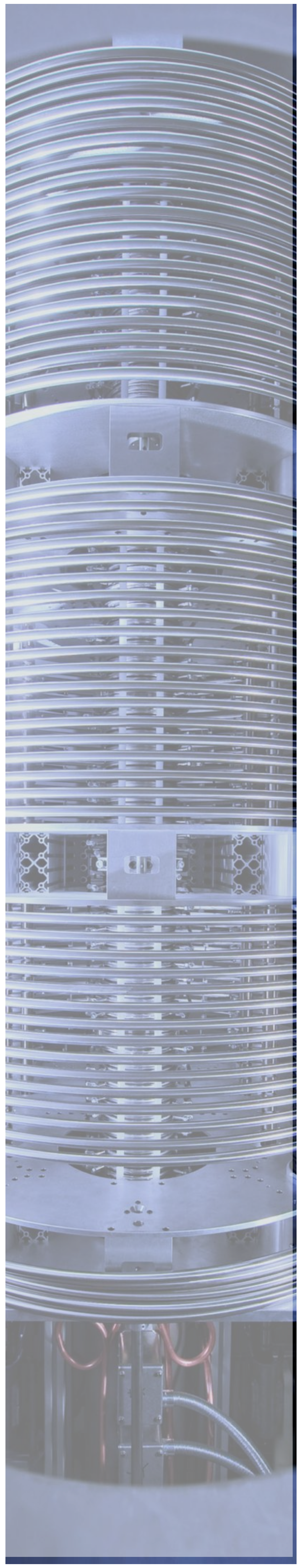

Abstract

Ab initio no-core configuration interaction (NCCI) calculations attempt to describe the structure of nuclei using realistic internucleon interactions. However, we can only describe these many-body systems within the limits of our computational power. As the number of nucleons increases, the calculations require more memory and processing power to reach convergence. Being able to accelerate convergence is crucial in extending the reach of NCCI calculations. Convergence can be obtained through a change of basis, for which we need to compute the overlaps of the radial functions for the new basis with those for the old basis. A large number of overlaps must be computed in order to accurately transform the many-body problem. Using alternative bases also requires the calculation of the one-body matrix elements for operators such as r^2 and p^2 in the new basis. We report a computer code that uses cubic spline interpolation to compute radial overlaps and radial integrals. This code facilitates using new bases to accelerate the convergence of NCCI calculations.

Computing the Overlaps

The integrals we want to evaluate can be highly oscillatory. They are given in the form of

$$\int_0^\infty f(r)dr \qquad (3)$$

First we must translate the bounds of the integration to an interval that is computational. We accomplish this with a simple change of variable that maps r from [0,infinity] to z from [0,1] .

This led us to the specific change of variable.

$$z = \frac{r}{r+1} \quad or\ equivalently \quad r = \frac{z}{1-z} \qquad (4)$$

$$Then\ dr = \frac{dz}{(1-z)^2} \qquad (5)$$

$$Yielding \int_0^\infty f(r)dr = \int_0^1 \frac{1}{(1-z)^2} f(\frac{z}{1-z})dz \qquad (6)$$

Once we have our integral on proper bounds. We can approximate the integrand using cubic spline interpolation. If we evaluate the integrand at n+1 points we can split the array of data points into n intervals. For each interval we can approximate the function between the interval with a polynomial.. Thus for i = 0,1,2...,n

$$S_i(x) = a_i(x-x_i)^3 + b_i(x-x_i)^2 + c_i(x-x_i) + d_i \qquad (7)$$

Now that we have an integrand that is smooth and a polynomial our integral becomes fast and simple.

No-Core Configuration Interaction Approaches

The no-core-shell model was developed as a non-perturbative approach to exactly solve nucleon-nucleon (NN) and NN + three-nucleon (NNN) interactions[1]. Traditionally the harmonic oscillator basis functions would serve as the basis for NCCI calculations. Unfortunately, the falloff of Gaussian functions at large r does not accurately describe the asymptotic features of the nuclear wave functions[1] This is where we are in luck. We can do a simple change of basis to the laguerre basis to yield the correct asymptotic features.

Matrix Elements for NCCI Calculations

To perform NCCI calculations we need two-body matrix elements of kinematic operators which can be broken down into one-body matrix elements. These one body matrix elements are given by

$$\langle R_{nl}|O|R_{\tilde{n}l}\rangle = \int_0^\infty dr R_{nl}(r) \times O \times R_{\tilde{n}l}(r) \qquad (1)$$

$$\text{where } O = r, r^2, p, p^2$$

$R_{nl}(r)$ represents the radial wavefunction of the harmonic oscillator at a given energy level n and orbital angular momentum l (Appendix 9.). These matrix elements can also be computed in momentum eigenspace, this is where p and p^2 operators come into play. The resulting radial integrals can be solved exactly through analytical methods. However this is tedious and extremely time consuming.

Accuracy and Speed

The largest factor in deciding our method of integration was accuracy, However this comes at the cost of time. Cubic spline interpolation brings the best of both worlds. Figure 2 shows us how accurate CSI can be with a few thousand data points. Figure 2. Plots the difference between the approximated value and the exact value of the integral. The computed value fluctuates violently until the approximation converges to the exact value at N = 700.

Although this is extremely oscillatory (97 roots) integral (n = 50 and n' = 47), CSI is able to obtain an approximation within 10^{-12} of the exact result. The only problem is that the calculation time is a linear function of spline intervals, meaning if we increase N 10 fold, then calculation time increases 10 fold. However at N = 700 a single integral takes less than a tenth of a second. Thankfully we only had to compute a couple thousand integrals, Meaning we can compute all necessary integrals at convergence within a single hour.

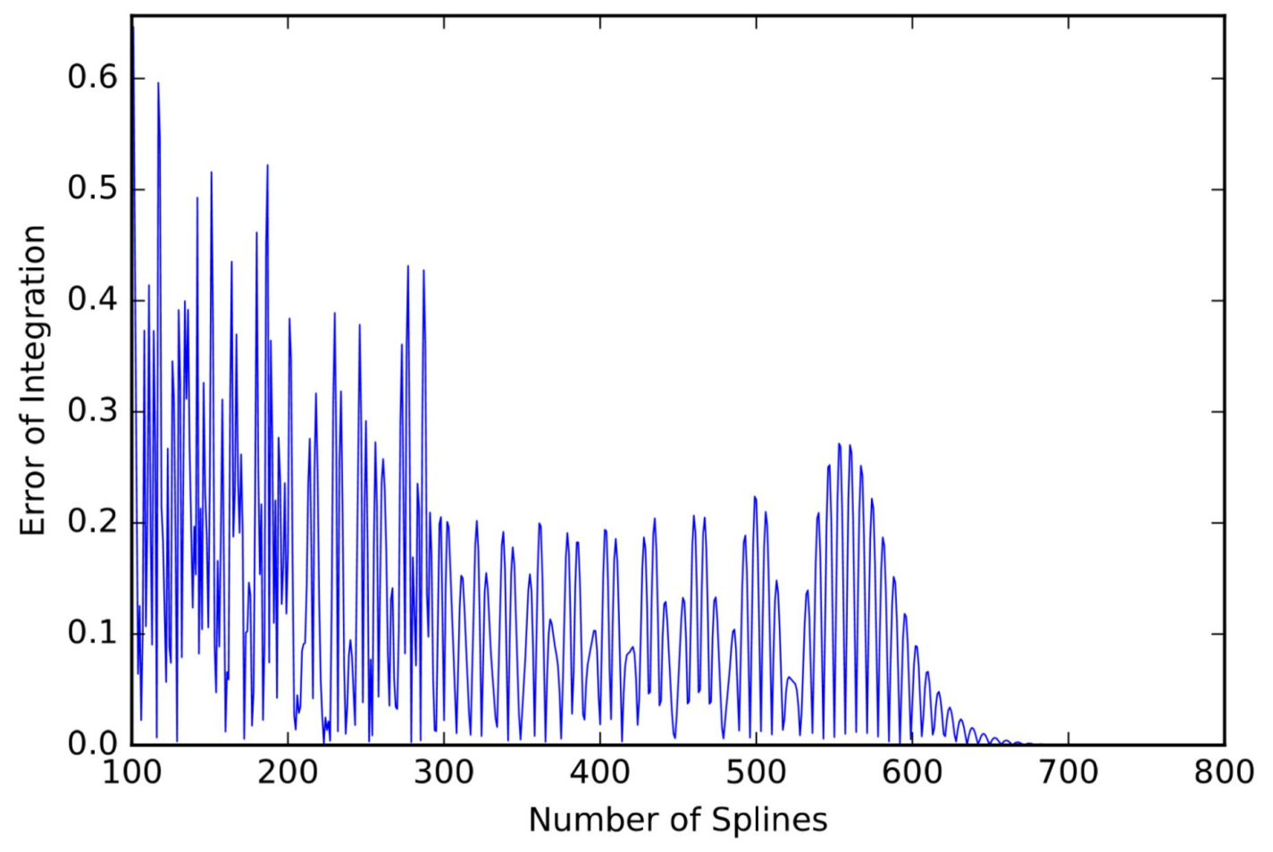

Figure 2. The convergence of

$$\int_0^\infty R_{50\,32}(r)R_{47\,32}(r)\,dr \qquad (8)$$

as a function of the number of splines

Transformation of Matrix Elements

Following the process outlined in [2] (Section III: C) In order to perform a change of basis from the old basis to our new basis we will need to compute the overlaps between the old and the new basis. These overlaps are given by

$$\langle R_{nl}|S_{\tilde{n}l}\rangle = \int_0^\infty dr R_{nl}(b_{HO};r)S_{\tilde{n}l}(b_l;r) \qquad (2)$$

$S_{nl}(r)$ represents the radial wavefunction in the Laguerre basis (Appendix 10.). As before these integrals can be calculated exactly through analytical methods. However, once again it is tedious and time consuming.

Figure 1. Shows us that the integrand of the integrals in the overlaps become extremely oscillatory quickly. Computationally this creates a problem for generic integration methods. As it is difficult for simpson's method or the trapezoid method to approximate extremely oscillatory integrals accurately. We are motivated to use a computational integration method that was both accurate and fast.

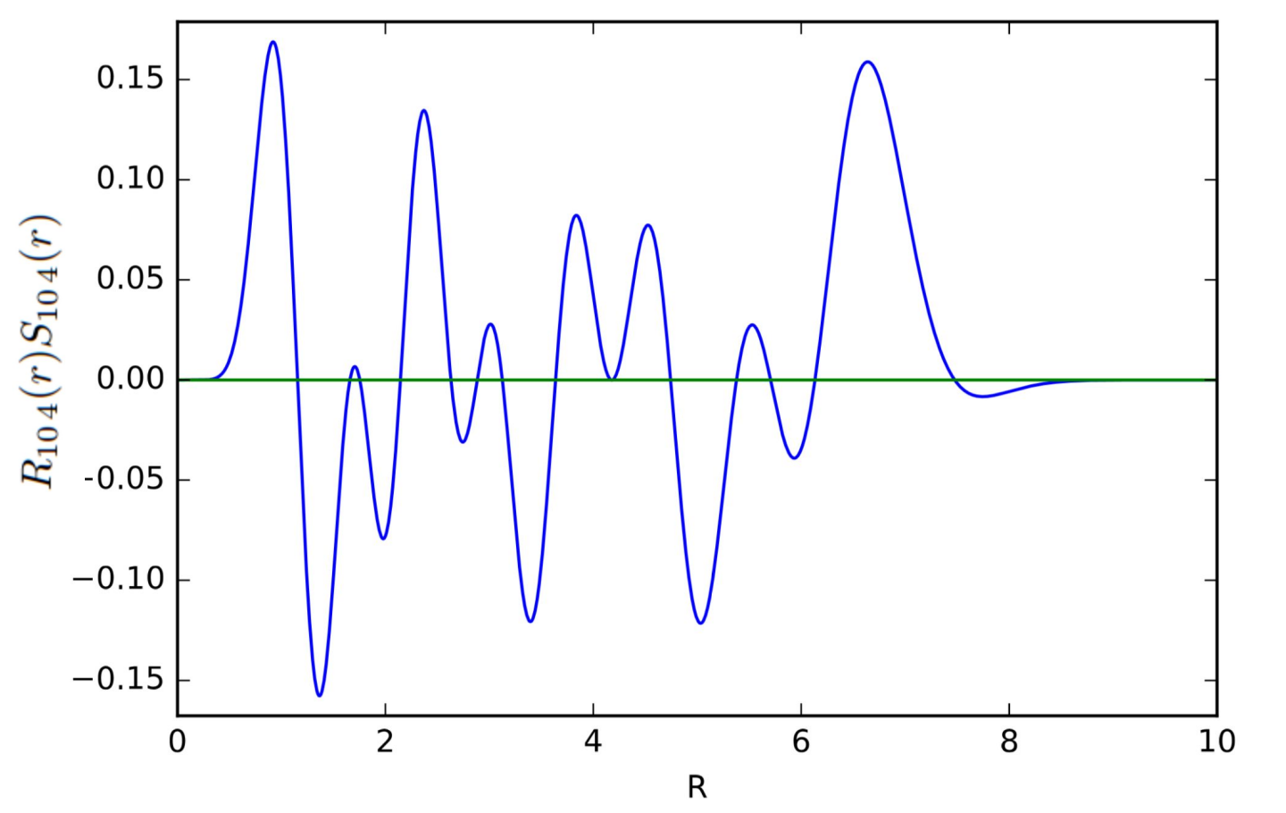

Figure 1. Evaluating $R_{10\,4}(r)S_{10\,4}(r)$ from r = 0 to r = 10

References

1. Barrett, Bruce R., Petr Navrátil, and James P. Vary. Ab initio no core shell model. Progress in Particle and Nuclear Physics 69 (2013): 131-181.
2. Caprio, M. A., P. Maris, and J. P. Vary. Coulomb-Sturmian basis for the nuclear many-body problem. Physical Review C 86.3 (2012): 034312.
3. Newman, Mark. Computational physics.CreateSpace Independent Publ., 2012.

Appendix

$$R_{nl}(r) = bN_{nl}(r/b)^{l+1}L_n^{l+1/2}[(r/b)^2]e^{-(r/b)^2/2}. \qquad N_{nl} = \frac{1}{b^{3/2}}\left[\frac{2\,n!}{(l+n+1/2)!}\right]^{1/2} \qquad (9)$$

$$S_{nl}(r) = (2/b)^{-1}N_{nl}(2r/b)^{l+1}L_n^{2l+2}(2r/b)e^{-r/b} \qquad N_{nl} = \left(\frac{2}{b}\right)^{3/2}\left[\frac{n!}{(n+2l+2)!}\right]^{1/2} \qquad (10)$$

Acknowledgments

Supported by the US NSF under grant NSF-PHY05-52843 the US DOE under grant DE-FG02-95ER-40934.

This project made use of computing resources provided by the Notre Dame Center for Research Computing

Conference Experience for Undergraduates (CEU), 2016 Fall Meeting of the APS Division of Nuclear Physics October 13-16, 2016, Vancouver, BC, Canada