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# Spectrum of few-body systems in a finite volume

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**Abstract.** Lattice quantum chromodynamics calculations of multi-baryon systems with physical quark masses could bridge the gap between nuclear physics and its fundamental theory. Such calculations are performed on a finite grid, and thus extrapolation of finite-volume numerical results to the physical-relevant free-space quantities is needed. A common approach for the extrapolation utilizes the two-body Lüscher formula and its generalization to larger systems. To understand better the accuracy of this approach we study here two model systems, bosonic and fermionic. The few-body systems are solved with the stochastic variational method in a periodic box, and the extrapolated values are compared to those calculated directly in free space.

## 1 Introduction

The underlying theory of the strong force is quantum chromodynamics (QCD), and thus it is of great interest to understand nuclear physics directly from QCD. *Ab initio* QCD predictions of few-nucleon systems can be achieved from numerical calculations on a finite lattice, known as lattice QCD (LQCD). Such calculations are performed with discrete spacing between lattice sites and in a finite volume with periodic boundary conditions. For infinitesimal spacing and infinite box size, LQCD provides an exact solution of QCD [1]. Since the box sizes in LQCD calculation are in the same length scale as the size of the wave function, an appropriate extrapolation method is required.

A popular method for extrapolating finite volume results to the physical free-space values utilizes the Lüscher formula [2], relevant for the two body case in the limit of short-range interaction and large boxes. A similar formula is valid also for few-body bound states, assuming that the asymptotic part of their wave function describes separation of the system into two subclusters, and treating each subcluster as a point-like particle [3].

The applicability of such an approach for light nuclei was studied recently in the framework of pionless effective field theory [4]. Here we expand this work by studying two other few-particle systems, namely spinless bosons interacting with local Gaussian interaction, as well as nucleons interacting with the Minnesota potential [5].

We perform few-body calculations in a periodic box and free space using a correlated Gaussians basis, which is optimized with the stochastic variational method (SVM) [6]. The resulting shifts in the binding energy induced by the finite volume are compared to the values predicted by the relevant formulae using parameters extracted directly from free-space calculations.

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## 2 Models and methods

The leading correction to the binding energy of a two-body $s$-wave bound state $\Delta B_2$, in the limit of large box size $L$, was derived by Lüscher [2],

$$\Delta B_2 = \frac{6\kappa_2|\mathcal{A}_2|^2}{\mu_2 L} e^{-\kappa_2 L}, \tag{1}$$

where $\mu_2$ is the reduced mass, $\kappa_2 = \sqrt{2\mu_2 B_2^{\text{free}}}$ is the binding momentum, and $\mathcal{A}_2$ is the dimensionless two-body asymptotic normalization coefficient (ANC). Here we use $\hbar = 1$.

A similar approach was used to analyze $N$-body bound states, once the lowest $s$-wave threshold of the system corresponds to a breakup into two subclusters, assuming that each of these subclusters behaves as a point-like particle. In this case, the leading correction is [3],

$$\Delta B_N = C_N \frac{6\kappa_N|\mathcal{A}_N|^2}{\mu_N L} e^{-\kappa_N L}, \tag{2}$$

where $\mu_N$ is the reduced mass of the subclusters and $\kappa_N = \sqrt{2\mu_N(B_N^{\text{free}} - B_a^{\text{free}} - B_b^{\text{free}})}$ is the binding momentum calculated from the free-space $N$-body binding energy $B_N^{\text{free}}$ and the binding energies $B_a^{\text{free}}$, $B_b^{\text{free}}$ of subclusters $a$ and $b$. Here, $C_N$ stands for a combinatorial factor that counts the number of options to partition $N$ particles into two subclusters and $\mathcal{A}_N$ denotes the ANC corresponding to the asymptotic part of the $N$-body wave function given by the inter-cluster coordinate. In principle, one should sum over corrections from all possible cluster configurations, however, the contribution of the lowest threshold is usually the dominant one.

Here, we study the finite-volume implications on two model cases. The first case is a system of a few spinless bosons interacting via local Gaussian potential,

$$V(r) = V_0 \exp(-r^2/R^2), \tag{3}$$

where the potential parameters, $V_0 = -5$ and $R = 1$, are taken from Ref. [3], and we work in the natural units where $m = 1$.

The second case represents a series of light nuclei with $A \leq 4$ nucleons interacting via the Minnesota nucleon-nucleon potential [5], with the exchange-mixture parameter $u = 1$. This spin-dependent interaction was fitted to reproduce nucleon-nucleon effective range parameters and gives reasonable binding energies for the deuteron, triton, and $^4$He nuclei treated here. In this work, we neglect the Coulomb interaction.

Considering only the ground states of the $s$-wave nuclei $^2$H, $^3$H, and $^4$He, we note that the lowest separation thresholds are those associated with breakup into $(N-1)$-particle subcluster and one nucleon. This is also the case for the bosonic system.

The binding energies and wave functions are solved numerically with the SVM. The $N$-body wave function is expanded in a correlated Gaussian basis, where the basis functions parameters are optimized to the system at hand in a stochastic way. Putting the system in a periodic box, the boundary conditions are enforced by including all possible shifts of the basis functions in an integer multiplication of the box size [7]. Our implementation of the SVM in a box is described in Ref. [8], while to enable fast and accurate calculations such as those presented here, a significant upgrade of the code was needed [4]. For more details see Refs. [4, 7, 8].

# 3 Results

## 3.1 Systems of few bosons

First, we show the energy shift due to the periodic box for the bosonic systems studied in Ref. [3]. The energy shifts for the $N = 2$, 3, and 4-body systems are shown as a function of the box sizes in figure 1. For large boxes, the results are in agreement with the Lüscher-like formulae, Eqs. (1) and (2). Both $\kappa_N$ and $\mathcal{A}_N$ were extracted from free-space calculations, and therefore no free parameter was used. For small boxes, however, significant deviations exist (note the log scale), and the validity of the asymptotic formulae deteriorates.

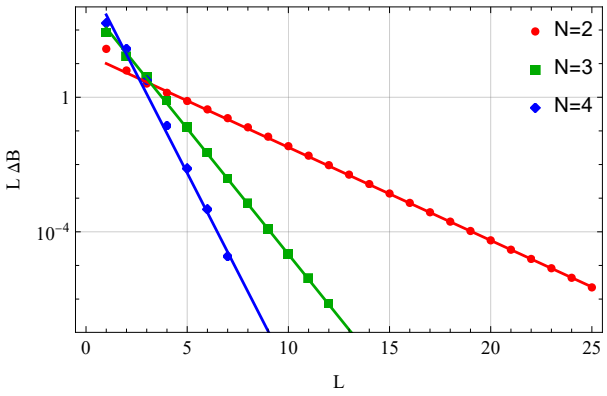


**Figure 1.** The energy shift $\Delta B_N$ due to the finite volume, multiplied by the box size $L$, as a function of $L$ for the bosonic case, in natural units. Shown are results for dimer (red), trimer (green), and tetramer (blue). The symbols represent SVM results, while the curves are the the Lüscher-like formulae, Eqs. (1,2) using free-space $\mathcal{A}_N$ and $\kappa_N$ values.

The binding energies and the ANCs for the bosonic systems are listed in table 1, and are compared to the results of Ref. [3]. Small differences between the values result from the fact that the kinetic energy was calculated in Ref. [3] with a finite difference scheme.

**Table 1.** Binding energies (in natural units) and dimensionless ANCs for the bosonic case, from Ref. [3] and as calculated here. ANCs are calculated by fitting the energy shifts in a box (fit), by the expectation value of a short-range operator (operator), and deduced directly from the free-space wave function (free).

| N | BE | | $\mathcal{A}_N$ | | | |
|---|---|---|---|---|---|---|
| | Ref. [3] | This work | Ref. [3] | | This work | |
| | | | fit | operator | fit | free |
| 2 | 0.449 | 0.4061 | 1.634(3) | 1.633(9) | 1.58(1) | 1.57682(1) |
| 3 | 2.916 | 2.6263 | 3.92(5) | 4.11(6) | 3.8(1) | 3.707(2) |
| 4 | – | 7.5135 | – | – | 8(2) | 6.99(1) |

## 3.2 Light nuclei

Now we move to the second case, i.e. light nuclei with the Minnesota potential. The energy shift in a box is shown in figure 2. For large boxes, the SVM results fit nicely the Lüscher-like formulae, Eqs. (1,2) using free-space $\mathcal{A}_N$ and $\kappa_N$ values. Also here we see significant differences for small boxes, showing the limitation of the asymptotic formulae.

The binding energies and the ANCs for light nuclei with the Minnesota nucleon-nucleon potential, as well as ANC values extracted from experiment results [9–11], are listed in table 2.

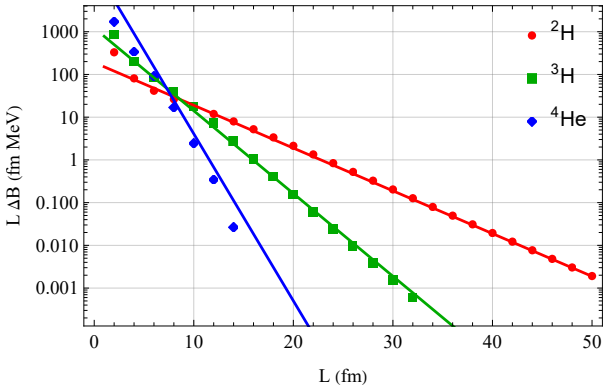


**Figure 2.** The energy shift $\Delta B_N$ due to the finite volume, multiplied by the box size $L$, as a function of $L$, for light nuclei using the Minnesota potential. Shown are results for deuteron (red), triton (green), and $^4$He (blue). Symbols represent SVM results, and curves are the predictions of Lüscher-like formulae, Eq. (1,2) using free-space $\mathcal{A}_N$ and $\kappa_N$ values.

**Table 2.** Binding energies (in MeV) and dimensionless ANCs of one nucleon separation for light nuclei. ANCs are calculated by fitting the energy shifts in a box (fit), deduced directly from the free-space wave function (free), and compared also to the values extracted from experiments (exp.).

| sys. | BE | $\mathcal{A}_N$ | | | |
|---|---|---|---|---|---|
| | (MeV) | fit | free | exp. | Ref. |
| $^2$H | 2.2023 | 1.3(1) | 1.28703 | 1.2902(65) | [9] |
| $^3$H | 8.3858 | 1.8(1) | 1.9145(1) | 2.19(2) | [10] |
| $^4$He | 30.782 | 4(1) | 5.265(3) | 4.11-6.42 | [11] |

## 4 Conclusion

Here we studied the accuracy of the formulae for the binding energy shift in a periodic box, and their applicability to extract free-space parameters, like the ANC, from finite-volume calculations. We explored two cases: a few bosons interacting via local Gaussian potential, and light nuclei with the Minnesota nucleon-nucleon interaction. In both cases, these formulae indeed give the leading correction, but quite large boxes are needed for performing accurate extrapolation.

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