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Improving the Volume Dependence of Two-Body Binding Energies Calculated with Lattice QCD

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Abstract

Volume modifications to the binding of two-body systems in large cubic volumes of extent L depend upon the total momentum and exponentially upon the ratio of L to the size of the boosted system. Recent work by Bour *et al* determined the momentum dependence of the leading volume modifications to nonrelativistic systems with periodic boundary conditions imposed on the single-particle wavefunctions, enabling them to numerically determine the scattering of such bound states using a low-energy effective field theory and Lüscher's finite-volume method. The calculation of bound nuclear systems directly from QCD using Lattice QCD has begun, and it is important to reduce the systematic uncertainty introduced into such calculations by the finite spatial extent of the gauge-field configurations. We extend the work of Bour *et al* from nonrelativistic quantum mechanics to quantum field theory by generalizing the work of Lüscher and of Gottlieb and Rummukainen to boosted two-body bound states. The volume modifications to binding energies can be exponentially reduced from $\mathcal{O}\left(e^{-\kappa L}/L\right)$ to $\mathcal{O}\left(e^{-2\kappa L}/L\right)$ in nonrelativistic systems (where κ is the binding momentum of the state) by forming particular combinations of the binding energies determined in the four lowest-lying boosted systems. Relativistic corrections to this combination, and others, that violate the exponential reduction are determined. An analysis of what can be expected from Lattice QCD calculations of the deuteron is performed, the results of which are representative of a generic loosely bound system.

I. INTRODUCTION

One of the major goals of nuclear physics research is to determine the properties and interactions of nucleons and nuclei, and more generally hadrons, directly from the underlying theory of the strong interactions, quantum chromodynamics (QCD). The only known way to accomplish this is to numerically evaluate the QCD path-integral using Lattice QCD (LQCD) in which the space-time continuum is replaced by a finite-volume grid, and the integrals over the fields at each point in space-time are performed using Monte-Carlo. The systematic errors introduced by a finite space-time volume, $L^3 \times T$, with a finite lattice spacing, b, can be systematically removed by performing calculations in multiple volumes, with multiple lattice spacings and using the theoretical knowledge of the associated functional dependences. The computational resources that are required for LQCD calculations with light quark masses (m_q) near their physical values, with small enough lattice spacings ($b\Lambda_\chi \ll 1$ where Λ_χ is the scale of chiral symmetry breaking), and in large enough lattice volumes ($m_\pi L \gtrsim 2\pi$) that permit reliable extrapolations and interpolations of phenomenologically important observables are now becoming available with the deployment of multi-peta-flop machines.

While calculating (post-dicting) the masses of the lowest-lying hadrons to high precision is computationally demanding (even without strong isospin breaking and electromagnetism), calculating the binding energies of systems composed of the lowest-lying hadrons (nuclei) to the same level of precision is significantly more demanding. For instance, calculating the mass of the proton at the percent level requires precision $\sim \pm 10$ MeV, while calculating the deuteron binding energy at the percent level requires precision of $\sim \pm 20$ keV. So while the same gauge-field configurations can be used for both calculations, the statistical precision required in the evaluation of the relevant correlation functions differs by orders of magnitude. Further, while the error in the calculation of a hadron mass introduced by the finite lattice volume scales as $\sim e^{-m_\pi L}$ for large volumes [1], the error in the calculation of a binding energy is largely dictated by the size of the bound state [1–3]. For instance, for a two-body bound state, the finite volume error scales as $\sim e^{-\kappa_0 L}/L$, where κ_0 is the binding momentum of the state, $B = -\left(\sqrt{m_1^2 - \kappa_0^2} + \sqrt{m_2^2 - \kappa_0^2} - m_1 - m_2\right)$, where B is the infinite-volume binding energy. For a loosely bound system such as the deuteron, the deviation between the ground-state energy calculated in a given LQCD calculation and the actual binding energy

will be dominated by the size of the deuteron [1] and will, in general, be significant except in very large volumes. These volume modifications arise from the exclusion of single-particle momentum modes in the bound state wavefunction due to the periodic boundary conditions (BC) that are imposed on the quark and gluon fields in the spatial directions.

During the last year, LQCD calculations have observed bound systems of baryons. Evidence for a bound H-dibaryon (a state with the quantum numbers of $\Lambda\Lambda$) was found in $n_f = 2 + 1$ LQCD calculations with $m_\pi \sim 390$ MeV [4, 5], and subsequent evidence was found in $n_f = 3$ calculations with $m_\pi \sim 840$ MeV [6]. Also, evidence was reported for ^{3}He, ^{4}He [7] and the deuteron [8] in quenched calculations with $m_\pi \sim 800$ MeV. The infinite volume binding energy for each of these nuclei was determined by calculating the ground state energy in a number ensembles of gauge-fields with different volumes and then extrapolating to infinite volume. While the generation of quenched gauge-fields is inexpensive computationally compared to the generation of QCD gauge-fields, the results of quenched calculations cannot be used to reliably predict quantities in nature.

An important observation that was recently made by Bour *et al* [9] in nonrelativistic systems is that the volume modifications depend upon the momentum of the bound state in the lattice volume, as moving bound states have different momentum modes excluded from their two-body wavefunction. The implication of this, when extended to quantum field theory, is that the unextrapolated binding energies of composite systems, and in particular light nuclei, calculated with LQCD will depend upon the total momentum of the system. Bour *et al* [9] were interested in calculating the scattering of bound states in a numerical evaluation of a low-energy effective field theory path integral, and found that the momentum dependent contribution to the two-body ground state energy had to be removed prior to using Lüscher's method [10, 11] to determine the phase-shift.

In this work, we extend the quantum field theory formalism established by Lüscher [10, 11] and generalized to moving systems by Rummukainen and Gottlieb [12], to determine the volume modifications of binding energies of bound systems composed of two spinless particles with s-wave interactions moving in a finite cubic volume, extending the results obtained by Bour *et al* [9] in nonrelativistic quantum mechanics. By forming combinations of the ground state energies of two-body systems with different lattice momenta, volume modifications can

[1] The modifications due to the non-zero range of the nuclear forces scale as $\sim e^{-m_\pi L}$.

be exponentially suppressed in the nonrelativistic limit, and we determine the violations of this exponential suppression. In the case of the deuteron, the lowest energy-eigenvalue in the np system with lattice momenta of $\mathbf{P} = \frac{2\pi}{L}\mathbf{d}$ with $|\mathbf{d}|^2 = 0, 1, 2, 3$ allow for the infinite-volume deuteron binding energy to be determined with a volume modification of $\Delta B^{(vol)} \lesssim 20$ keV for $L \gtrsim 12$ fm, orders of magnitude smaller than in the ground state energy of the $|\mathbf{d}| = 0$ system alone. From a practical standpoint, forming such linear combinations of boosted ground state energies requires significantly smaller computational resources than computing the ground state energies in multiple lattice volumes. The former can be accomplished with one set of quark propagators on one ensemble of gauge fields, while the later requires generating multiple ensembles of gauge fields and quark propagators on each. In some sense, these linear combinations of binding energies represent an exponential "volume-improvement" of the binding energy calculation on a given ensemble of gauge-fields.

An analysis of possible determinations of the deuteron binding energy from a single lattice volume was carried out in Ref. [13]. For a large enough lattice volume, the energies of the lowest two levels with $|\mathbf{d}| = 0$ fall below the t-channel cut, and the effective range expansion (ERE) of $p \cot \delta$ can be used. Truncating the ERE at the first two terms, which is known to be a good approximation for nucleon-nucleon scattering, allows the deuteron binding energy to be obtained by an interpolation. Of course, it is desirable to not make such an approximation in extracting the deuteron binding energy, but this would require more states below the t-channel cut and hence even larger lattice volumes.

II. SPINLESS PARTICLES WITH S-WAVE INTERACTIONS

For spinless particles of mass m_1 and m_2 interacting in an s-wave, the scattering amplitude below the inelastic threshold is uniquely specified by the phase-shift δ_0, and is proportional to $1/(q^* \cot \delta_0 - iq^*)$ where q^* is the magnitude of the momentum of each particle in the center-of-momentum (CoM) frame. When these two particles are confined to a cubic volume of spatial extent L subject to periodic BC's, and with total momentum $\mathbf{P} = \frac{2\pi}{L}\mathbf{d}$, the energy-eigenvalues of the system are the solutions to (when the formalism developed in Refs. [10–12, 14, 15] is generalized to systems of unequal mass particles, as outlined in the

appendix) [2]

$$q^* \cot \delta(q^*) \;=\; \frac{2}{\gamma L \sqrt{\pi}}\; Z_{00}^{(\mathbf{d})}(1; \tilde{q}^{*2}, \tilde{\Delta} m_{12}^2) \quad , \tag{1}$$

where

$$Z_{LM}^{(\mathbf{d})} \;=\; \sum_{\mathbf{r}} \frac{|\mathbf{r}|^L\; Y_{LM}(\Omega_{\mathbf{r}})}{|\mathbf{r}|^2 - \tilde{q}^{*2}} \quad , \quad \mathbf{r} \;=\; \frac{1}{\gamma}\left(\mathbf{n}_{\parallel} - \alpha \mathbf{d}\right) + \mathbf{n}_{\perp} \;=\; \hat{\gamma}^{-1}\left(\mathbf{n} - \alpha \mathbf{d}\right) \quad , \tag{2}$$

where $\mathbf{n}$ is a triplet of integers. A " * " denotes a quantity determined in the CoM frame, and for a system with $\mathbf{P} = \frac{2\pi}{L}\mathbf{d}$ and total energy E, the energy in the CoM frame is $s = E^{*2} = E^2 - |\mathbf{P}|^2$ which defines the γ-factor (which depends explicitly on $\mathbf{d}$), $\gamma = E/E^*$. The magnitude of the three-momentum in the CoM frame, q^*, is determined by $E^{*2} = (\sqrt{q^{*2} + m_1^2} + \sqrt{q^{*2} + m_2^2})^2$ and the factor α that appears in eq. (2) is

$$\alpha \;=\; \frac{1}{2}\left[1 \;+\; \frac{m_1^2 - m_2^2}{E^{*2}}\right] \quad . \tag{3}$$

In eq. (1), Δm_{12}^2 is defined as $\Delta m_{12}^2 = m_1^2 - m_2^2$, and a tilde over any variable denotes scaling by a factor of $L/(2\pi)$, e.g. $\tilde{q}^* = q^* L/(2\pi)$. In the case of equal masses ($m_1 = m_2$) $\alpha = \frac{1}{2}$, and the expressions in eq. (1) and eq. (2) reduce to the known result for boosted systems of equal mass [12, 14, 15]. Further developments are required in order to recover the results obtained for nonrelativistic systems by Bour *et al* from eq. (1), eq. (2) and eq. (3), as we now describe.

Assuming the scattering amplitude admits a single bound state in infinite volume, the location of the lowest energy-eigenvalue in a finite cubic volume is dictated by the behavior of $Z_{LM}^{(\mathbf{d})}$ for $\tilde{q}^{*2} < 0$. It is clear from the form of $Z_{LM}^{(\mathbf{d})}$ in eq. (2) that there are no poles along the negative axis, and the Poisson resummation formula can be used to determine its asymptotic behavior at large $-\tilde{q}^{*2}$. It is straightforward to show that for $q^{*2} < 0$

$$Z_{00}^{(\mathbf{d})}(1; \tilde{q}^{*2}, \tilde{\Delta} m_{12}^2) \;\to\; \frac{\gamma}{\sqrt{4\pi}}\left[\; -2\pi^2 \sqrt{-\tilde{q}^{*2}} \;+\; \sum_{\mathbf{m} \neq \mathbf{0}} \frac{\pi}{|\hat{\gamma}\mathbf{m}|}\; e^{i 2\pi \alpha \mathbf{m}\cdot\mathbf{d}}\; e^{-2\pi |\hat{\gamma}\mathbf{m}| \sqrt{-\tilde{q}^{*2}}}\right] \quad , \tag{4}$$

where

$$\hat{\gamma}\mathbf{m} \;=\; \gamma \mathbf{m}_{\parallel} + \mathbf{m}_{\perp} \;=\; (\gamma - 1)\frac{\mathbf{m}\cdot\mathbf{d}}{|\mathbf{d}|^2}\; \mathbf{d} \;+\; \mathbf{m} \quad , \tag{5}$$

[2] Exponentially suppressed corrections to this relation for $\pi\pi$ and NN scattering of the form $e^{-m_\pi L}$ have been determined in Ref. [16] and Ref. [17], respectively.

and the $\mathbf{m}$ are triplets of integers. By setting $q^* = i\kappa$, the eigenvalue equation in eq. (1) becomes

$$p \cot \delta(p)|_{p=i\kappa} \; + \; \kappa \; = \; \frac{1}{L} \sum_{\mathbf{m} \neq \mathbf{0}} \frac{1}{|\hat{\gamma}\mathbf{m}|} \, e^{i2\pi\alpha \mathbf{m}\cdot\mathbf{d}} \, e^{-|\hat{\gamma}\mathbf{m}|\kappa L} \; = \; \frac{1}{L} \, F^{(\mathbf{d})}(\kappa L) \quad . \tag{6}$$

In the infinite volume limit $F^{(\mathbf{d})}(\kappa L) = 0$, and the eigenvalue equation becomes

$$p \cot \delta(p)|_{p=i\kappa_0} \; + \; \kappa_0 \; = \; 0 \quad , \tag{7}$$

which correctly reproduces the location of the pole in the S-matrix. While it is not required for this analysis, below the t-channel cut $p \cot \delta(p)$ can be expanded in powers of the CoM energy $p \cot \delta(p) = -\frac{1}{a} + \frac{1}{2} r p^2 + ...$, defining the ERE, where a is the scattering length and r is the effective range. For the lowest few $\mathbf{d}$ vectors, the finite volume functions $F^{(\mathbf{d})}(\kappa L)$ are (where we keep in mind that γ depends upon $|\mathbf{d}|$)

$$\begin{aligned}
F^{(0,0,0)}(\kappa L) \; &= \; 6 \, e^{-\kappa L} \; + \; 6\sqrt{2} \, e^{-\sqrt{2}\kappa L} \; + \; \frac{8}{\sqrt{3}} \, e^{-\sqrt{3}\kappa L} \; + \; 3 \, e^{-2\kappa L} \; + \; ... \\
F^{(0,0,1)}(\kappa L) \; &= \; 2 \left(\; 2 \, e^{-\kappa L} \quad + \; \frac{\cos(2\pi\alpha)}{\gamma} e^{-\gamma\kappa L} \; \right) \\
&\quad + \; 2\sqrt{2} \left(\; e^{-\sqrt{2}\kappa L} \; + \; 2\cos(2\pi\alpha) \sqrt{\frac{2}{\gamma^2+1}} \, e^{-\sqrt{\gamma^2+1}\kappa L} \right) \\
&\quad + \; \frac{8\cos(2\pi\alpha)}{\sqrt{\gamma^2+2}} e^{-\sqrt{\gamma^2+2}\kappa L} \; + \; \left(\; 2 \, e^{-2\kappa L} \quad + \; \frac{\cos(4\pi\alpha)}{\gamma} e^{-2\gamma\kappa L} \; \right) \; + \; ... \\
F^{(0,1,1)}(\kappa L) \; &= \; 2 \left(\; e^{-\kappa L} \quad + \; 2\cos(2\pi\alpha) \sqrt{\frac{2}{\gamma^2+1}} e^{-\sqrt{\frac{\gamma^2+1}{2}}\kappa L} \; \right) \\
&\quad + \; \sqrt{2} \; \left(\; e^{-\sqrt{2}\kappa L} \; + \; \frac{\cos(4\pi\alpha)}{\gamma} \, e^{-\sqrt{2}\gamma\kappa L} \; + \; \frac{8\cos(2\pi\alpha)}{\sqrt{3+\gamma^2}} \, e^{-\sqrt{\frac{3+\gamma^2}{2}}\kappa L} \; \right) \\
&\quad + \; \frac{4}{\sqrt{3}} \left(\; e^{-\sqrt{3}\kappa L} \; + \; \cos(4\pi\alpha) \sqrt{\frac{3}{2\gamma^2+1}} e^{-\sqrt{2\gamma^2+1}\kappa L} \right) \\
&\quad + \; \left(\; e^{-2\kappa L} \quad + \; 2\cos(4\pi\alpha) \sqrt{\frac{2}{\gamma^2+1}} e^{-2\sqrt{\frac{\gamma^2+1}{2}}\kappa L} \; \right) + \; ... \\
F^{(1,1,1)}(\kappa L) \; &= \; 6\cos(2\pi\alpha) \sqrt{\frac{3}{\gamma^2+2}} e^{-\sqrt{\frac{\gamma^2+2}{3}}\kappa L} \\
&\quad + \; 3\sqrt{2} \left(\; e^{-\sqrt{2}\kappa L} \; + \; \cos(4\pi\alpha) \sqrt{\frac{3}{2\gamma^2+1}} \, e^{-\sqrt{\frac{2}{3}(2\gamma^2+1)}\kappa L} \; \right) \\
&\quad + \; \frac{2}{\sqrt{3}} \left(\frac{\cos(2\pi\alpha)}{\gamma} e^{-\sqrt{3}\gamma\kappa L} \; + \; \cos(6\pi\alpha) \, \frac{9}{\sqrt{\gamma^2+8}} e^{-\sqrt{\frac{\gamma^2+8}{3}}\kappa L} \right) \\
&\quad + \; 3\cos(4\pi\alpha) \sqrt{\frac{3}{\gamma^2+2}} e^{-2\sqrt{\frac{\gamma^2+2}{3}}\kappa L} \; + \; ... \quad ,
\end{aligned} \tag{8}$$

where the ellipses denotes terms that scale as $\sim e^{-\sqrt{5}\kappa_0 L}/L$ and higher. In the large volume limit where the $F^{(\mathbf{d})}$ will give rise to $\kappa^{(\mathbf{d})}$ that are close to κ_0, the $\kappa^{(\mathbf{d})}$ can be determined in a perturbative solution to eq. (6). Introducing the dimensionless parameter λ, writing $\kappa^{(\mathbf{d})} = \kappa_0 + \lambda\kappa_1^{(\mathbf{d})} + \lambda^2\kappa_2^{(\mathbf{d})} + ...$ along with the substitution $F^{(\mathbf{d})}(\kappa^{(\mathbf{d})}L) \to \lambda F^{(\mathbf{d})}(\kappa^{(\mathbf{d})}L)$ and equating orders in λ, leads to

$$\begin{aligned}
\kappa_1^{(\mathbf{d})} &= \frac{Z_\psi^2}{L}\, F^{(\mathbf{d})}(\kappa_0 L) \\
\kappa_2^{(\mathbf{d})} &= Z_\psi^2 \left(\kappa_1 \frac{1}{L}\frac{d}{d\kappa} F^{(\mathbf{d})}(\kappa_0 L) \;+\; \kappa_1^2 \frac{d}{dp^2} p\cot\delta|_{i\kappa_0} \;-\; 2\kappa_0^2\kappa_1^2 \frac{d^2}{(dp^2)^2} p\cot\delta|_{i\kappa_0} \right) \\
Z_\psi &= \frac{1}{\sqrt{1 - 2\kappa_0 \frac{d}{dp^2} p\cot\delta|_{i\kappa_0}}} \,,
\end{aligned} \tag{9}$$

where Z_ψ^2 is the residue of the bound-state pole in the S-matrix, and the higher $\kappa_i^{(\mathbf{d})}$ can be determined in a similar way. For a given boost-vector, $\kappa_1^{(\mathbf{d})}$ scales as $\kappa_1^{(\mathbf{d})} \sim e^{-\kappa_0 L}/L$ and $\kappa_2^{(\mathbf{d})}$ scales as $\kappa_2^{(\mathbf{d})} \sim e^{-2\kappa_0 L}/L$. Consequently, the contributions to $\kappa^{(\mathbf{d})}$ that scale as $\sim e^{-\kappa_0 L}/L$, $\sim e^{-\sqrt{2}\kappa_0 L}/L$ and $\sim e^{-\sqrt{3}\kappa_0 L}/L$ originate in $\kappa_1^{(\mathbf{d})}$ and are of the forms given in eq. (8).

It is clear from the explicit expressions for $F^{(\mathbf{d})}(\kappa L)$ given in eq. (8) that linear combinations that provide universal cancellations of finite volume effects in binding energies do not exist in general. This is due to the appearances of both γ-factors and α-factors that explicitly depend upon $\mathbf{d}$. However, the nonrelativistic (NR) limit where $\gamma = \gamma^{(\mathrm{NR})} = 1$ and neglecting the binding energy compared to the rest mass of the constituent hadrons, $\alpha = \alpha^{(\mathrm{NR})} = m_1/(m_1 + m_2)$, allows for relations to be constructed for a given value of $\alpha^{(\mathrm{NR})}$. Corrections to the relations can then be constructed as an expansion in $\gamma - \gamma^{(\mathrm{NR})}$ and $\alpha - \alpha^{(\mathrm{NR})}$. The case of equal masses, $m_1 = m_2$, is special because $\alpha = \frac{1}{2}$ for any binding energy and not just in the limit where the binding energy is small compared to the rest masses. In the NR limit it is useful to write

$$F^{(\mathbf{d})}(\kappa L) \;\to\; \sum_j \; f_j^{(\mathbf{d})(\alpha^{(\mathrm{NR})})} \; \frac{e^{-\sqrt{j}\kappa L}}{\sqrt{j}} \,, \tag{10}$$

where the coefficients $f_j^{(\mathbf{d})(\alpha^{(\mathrm{NR})})}$ for the case of equal masses, $m_1 = m_2$ with $\alpha^{(\mathrm{NR})} = \frac{1}{2}$, are given in Table I and the case where $m_2 = 2m_1$ with $\alpha^{(\mathrm{NR})} = \frac{1}{3}$ is given in Table II. The ratios of coefficients in $f_1^{(\mathbf{d})(\frac{1}{3})}$ column in Table II reproduce the quantity $\tau(\mathbf{k}, \frac{1}{3})$ that are tabulated in Table 1 in Ref. [9].

It is also worth pointing out that the ground state energy of the unboosted, $|\mathbf{d}| = 0$, equal-mass, $\alpha = \frac{1}{2}$, system has leading and subleading volume corrections that are three

TABLE I: The coefficients $f_j^{(\mathbf{d})(\frac{1}{2})}$ in eq. (10) that determine the leading four finite-volume corrections to the two-body binding energy in the nonrelativistic limit for a system with $m_1 = m_2$.

$\lvert\mathbf{d}\rvert^2$	$f_1^{(\mathbf{d})(\frac{1}{2})}$	$f_2^{(\mathbf{d})(\frac{1}{2})}$	$f_3^{(\mathbf{d})(\frac{1}{2})}$	$f_4^{(\mathbf{d})(\frac{1}{2})}$
0	6	12	8	6
1	2	−4	−8	6
2	−2	−4	8	6
3	−6	12	−8	6

TABLE II: The coefficients $f_j^{(\mathbf{d})(\frac{1}{3})}$ in eq. (10) that determine the leading four finite-volume corrections to the two-body binding energy in the nonrelativistic limit for a system with $m_2 = 2m_1$.

$\lvert\mathbf{d}\rvert^2$	$f_1^{(\mathbf{d})(\frac{1}{3})}$	$f_2^{(\mathbf{d})(\frac{1}{3})}$	$f_3^{(\mathbf{d})(\frac{1}{3})}$	$f_4^{(\mathbf{d})(\frac{1}{3})}$
0	6	12	8	6
1	3	0	−4	3
2	0	−3	2	0
3	−3	3	5	−3

times larger than those of the $|\mathbf{d}| = 1$ and $|\mathbf{d}| = \sqrt{2}$ systems. So while it does not constitute an exponential reduction in the volume modifications, the binding energy of the $|\mathbf{d}| = 1$ and $|\mathbf{d}| = \sqrt{2}$ systems will be significantly closer to the infinite volume binding energy than that of the $|\mathbf{d}| = 0$ system.

A. Volume-Improvement for Equal Mass Systems : $\alpha = \frac{1}{2}$

The equal mass systems are special, as mentioned previously, because $\alpha = \frac{1}{2}$ is independent of the binding energy of the system, a feature that is not present for $m_1 \neq m_2$. Using the coefficients in Table I it is straightforward to construct relations that eliminate the leading and subleading orders of the volume modifications. We consider five relations:

$$\begin{aligned}\overline{\kappa}^A &= \frac{1}{8}\Big(\ \kappa^{(0,0,0)} \ + \ 3\kappa^{(0,0,1)} \ + \ 3\kappa^{(0,1,1)} \ + \ \kappa^{(1,1,1)}\ \Big) \\ &= \kappa_0 \ + \ \frac{3Z_\psi^2}{2L}\ \eta^2 \ \left(1+\kappa_0 L\right) e^{-\kappa_0 L} \ + \ \mathcal{O}\left(\eta^4 e^{-\kappa_0 L} L, \frac{e^{-2\kappa_0 L}}{2L}\right)\end{aligned}$$

$$
\begin{aligned}
\overline{\kappa}^B &= \frac{1}{4}\Big(\ \kappa^{(0,0,0)} \ + \ 3\kappa^{(0,1,1)}\Big) \\
&= \kappa_0 \ + \ \frac{3Z_\psi^2}{2L}\eta^2 \ \left(1+\kappa_0 L\right) e^{-\kappa_0 L} \ + \ \mathcal{O}\left(\eta^4 e^{-\kappa_0 L} L, \frac{e^{-\sqrt{3}\kappa_0 L}}{\sqrt{3}L}\right) \\
\overline{\kappa}^C &= \frac{1}{4}\Big(\ \kappa^{(1,1,1)} \ + \ 3\kappa^{(0,0,1)}\Big) \\
&= \kappa_0 \ + \ \frac{3Z_\psi^2}{2L}\eta^2 \ \left(1+\kappa_0 L\right) e^{-\kappa_0 L} \ + \ \mathcal{O}\left(\eta^4 e^{-\kappa_0 L} L, \frac{e^{-\sqrt{3}\kappa_0 L}}{\sqrt{3}L}\right) \\
\overline{\kappa}^D &= \frac{1}{4}\Big(\ \kappa^{(0,0,0)} \ + \ \kappa^{(0,0,1)} \ + \ \kappa^{(0,1,1)} \ + \ \kappa^{(1,1,1)} \ \Big) \\
&= \kappa_0 \ + \ \frac{3Z_\psi^2}{2L}\ \eta^2 \ \left(1+\kappa_0 L\right) e^{-\kappa_0 L} \ + \ \mathcal{O}\left(\eta^4 e^{-\kappa_0 L} L, \frac{e^{-\sqrt{2}\kappa_0 L}}{\sqrt{2}L}\right) \\
\overline{\kappa}^E &= \frac{1}{2}\Big(\ 3\kappa^{(0,0,1)} \ - \ \kappa^{(0,0,0)} \ \Big) \\
&= \kappa_0 \ + \ \frac{3Z_\psi^2}{2L}\ \eta^2 \ \left(1+\kappa_0 L\right) e^{-\kappa_0 L} \ + \ \mathcal{O}\left(\eta^4 e^{-\kappa_0 L} L, \frac{e^{-\sqrt{2}\kappa_0 L}}{\sqrt{2}L}\right) \ , \qquad (11)
\end{aligned}
$$

where $\gamma^2 = 1 + \eta^2 |\mathbf{d}|^2$ with $\eta = \frac{2\pi}{LE^*}$. From the forms of the volume expansions given in eq. (11), we see that $\overline{\kappa}^A$ eliminates the largest three volume contributions up to relativistic corrections, while $\overline{\kappa}^B$ and $\overline{\kappa}^C$ eliminate the first two contributions, and $\overline{\kappa}^D$ and $\overline{\kappa}^E$ eliminate only the first.

III. NUMERICAL EXPLORATION OF THE DEUTERON BINDING ENERGY

The deuteron is the simplest nucleus, comprised of a neutron and a proton. Its binding energy is $B = 2.224644(34)$ MeV which corresponds to a binding momentum of $\kappa_0 \sim 45.70$ MeV (using the isospin averaged nucleon mass of $M_N = 938.92$ MeV). As it is a spin-1 system composed of two spin-$\frac{1}{2}$ nucleons, its wavefunction is an admixture of s-wave and d-wave. The system is predominantly s-wave with a small admixture of d-wave induced by the tensor ($L = S = 2$) interaction. For the purposes of this analysis we will neglect the small d-wave admixture in the deuteron wavefunction and assume that the deuteron is entirely s-wave. The low-energy s-wave scattering of a neutron and proton with $J^\pi = 1^+$ is well described by effective range theory, where the ERE of $p \cot \delta$ converges rapidly with just the first two terms. The scattering length is known to be $a^{(^3S_1)} = 5.425(1)$ fm, the effective range is $r^{(^3S_1)} = 1.749(8)$ fm, and the shape parameter is anomalously small and neglected. The central values of these two parameters in the s-wave amplitude give rise to a deuteron

binding energy of $B \sim 2.212$ MeV with a corresponding κ_0 of $\kappa_0 \sim 45.58$ MeV, which are within $\sim 0.5\%$ of the actual deuteron binding parameters.

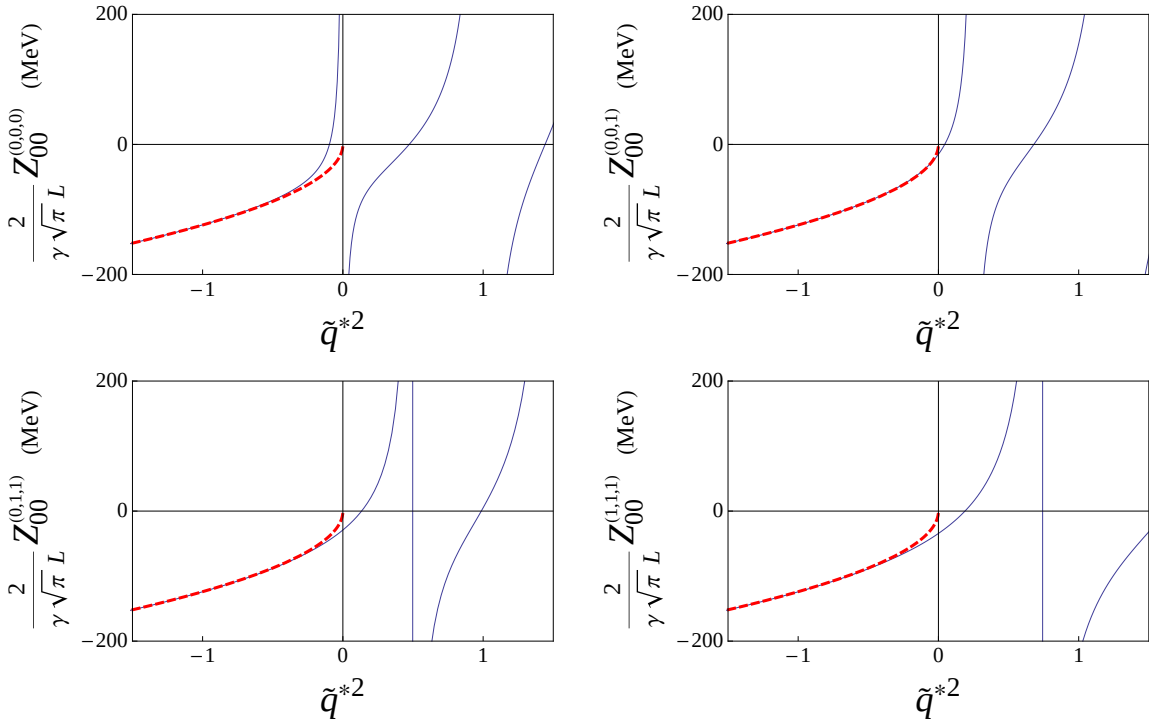

FIG. 1: The $Z_{00}^{(\mathbf{d})}(1;\tilde{q}^{*2},0)$ functions (blue curves), normalized by $\frac{2}{\gamma L\sqrt{\pi}}$, for the deuteron in a cubic volume with $L = 10$ fm. The dashed (red) curves correspond to $-\sqrt{-\tilde{q}^{*2}}$, asymptotic form of the function as $\tilde{q}^{*2} \to -\infty$. The hyperfine splitting of the lowest poles in the $|\mathbf{d}|^2 = 2, 3$ functions, determined by $\gamma - 1$, is evident.

The functions $\frac{2}{\gamma L\sqrt{\pi}} Z_{00}^{(\mathbf{d})}(1;\tilde{q}^{*2},0)$ for $|\mathbf{d}|^2 = 0, 1, 2, 3$ are shown in fig. 1, along with their asymptotic form $-\sqrt{-\tilde{q}^{*2}}$ at large $-\tilde{q}^{*2}$. It is clear that, of the four functions shown, the $|\mathbf{d}| = 0$ function will give rise to the largest volume modifications to the deuteron binding energy, as reflected in the deviation from its asymptotic form. This is because this function has a pole at $\tilde{q}^{*2} = 0$, while the $|\mathbf{d}|^2 = 1, 2, 3$ functions do not. It is also clear from fig. 1, and magnified in fig. 2, that the $|\mathbf{d}| = 1$ function exhibits the smallest deviations from its asymptotic form and the volume modifications to the deuteron binding are expected to be the smallest of the four considered. An interesting point to note from fig. 2 is that despite $Z_{00}^{(0,0,1)}$ having volume modifications that start at $\mathcal{O}\left(e^{-\kappa L}/L\right)$, there are significant cancellations between all of the exponential contributions, leaving the function very close to its asymptotic value over most of the range of κ. Figure 3 shows the ground state energy in

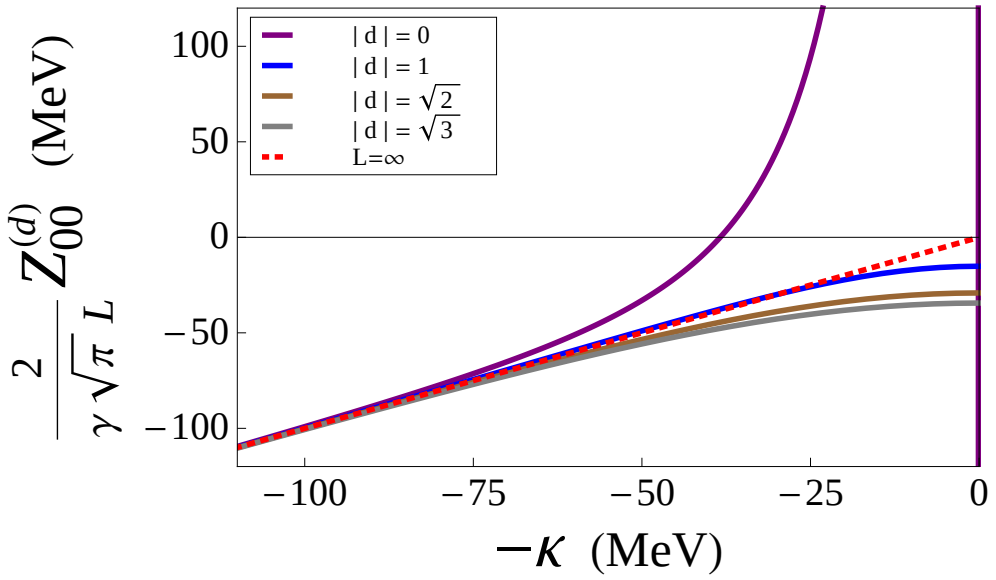

FIG. 2: The $\frac{2}{\gamma L\sqrt{\pi}} Z_{00}^{(\mathbf{d})}(1;\tilde{q}^{*2},0)$ functions appearing in eq. (1) for a deuteron with momentum $\mathbf{P} = \frac{2\pi}{L}\mathbf{d}$ for $|\mathbf{d}|^2 = 0,1,2,3$ in a cubic volume with $L = 10$ fm evaluated at $\tilde{q}^{*2} = -\kappa^2 \frac{L^2}{4\pi^2}$. The dotted (red) curve corresponds to extrapolating the $L \to \infty$ asymptotic forms of the functions, $-\kappa$.

the deuteron channel (negative of the binding energy) as a function of the spatial extent of the volume through numerical solution of eq. (6). Also shown in this figure are the contributions from the $\mathcal{O}\left(e^{-\kappa_0 L}/L\right)$ volume modifications, and from the volume modifications up to and including $\mathcal{O}\left(e^{-\sqrt{3}\kappa_0 L}/L\right)$.

Forming the linear combinations of the $\kappa^{(\mathbf{d})}$ given in eq. (11), the $\overline{\kappa}^i$, from the exact numerical solutions to eq. (6), gives rise to the improved estimates of the deuteron binding energy that are shown in fig. 4. Surprisingly, there is little difference between the volume modifications improved to $\mathcal{O}\left(e^{-2\kappa_0 L}/L\right)$ and those improved to $\mathcal{O}\left(e^{-\sqrt{3}\kappa_0 L}/L\right)$ for volumes with 10 fm$\lesssim L\lesssim$ 20 fm. For $L\gtrsim$ 12 fm the $\overline{\kappa}^i$, except for $\overline{\kappa}^E$, provide estimates of the deuteron binding energy that are significantly closer to its actual binding energy than the ground state of any given $\mathbf{d}$ spectrum. The $\overline{\kappa}^D$ combination is closer to the infinite volume binding energy than one would expect. While it is improved to $\mathcal{O}\left(e^{-\sqrt{2}\kappa_0 L}/L\right)$ it appears to be better than any of the others that are improved to higher orders. However, this is true only at these "intermediate" volumes, while in the very large volumes the predicted hierarchy is, in fact, found, as seen in the right panel of fig. 4. In this combination there is a

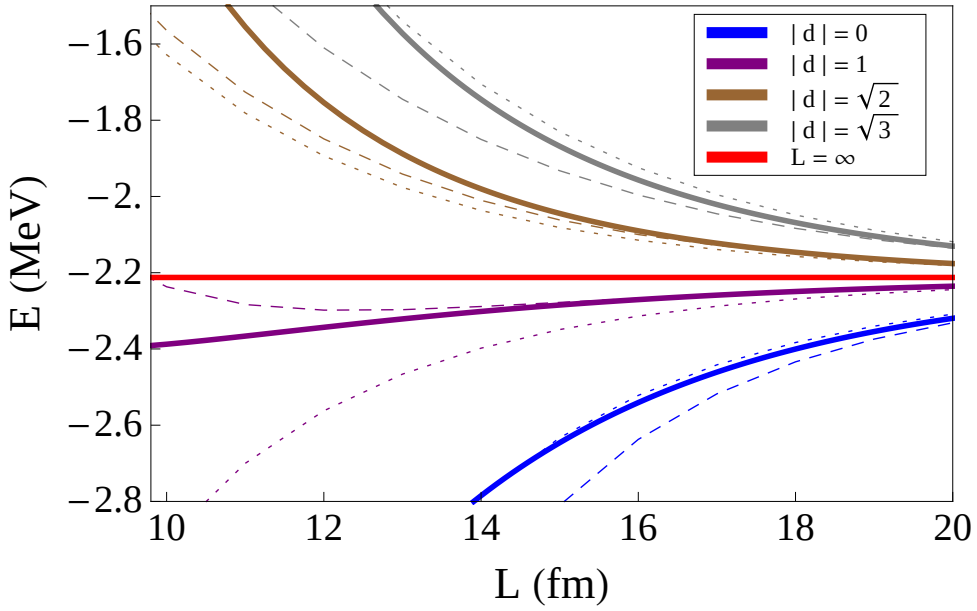

FIG. 3: The ground state energy in the deuteron channel. The blue, purple, brown and gray solid curves are the exact energies of the ground state of the system with total momentum $\mathbf{P} = \frac{2\pi}{L}\mathbf{d}$, determined in eq. (6). The solid red line is the infinite volume ground state energy. The dotted curves result from the analytic forms of the volume modifications truncated at $\mathcal{O}\left(e^{-\kappa_0 L}/L\right)$, given in eq. (8) using the coefficients in table I, while the dashed curves result from the analytic forms truncated at $\mathcal{O}\left(e^{-\sqrt{3}\kappa_0 L}/L\right)$.

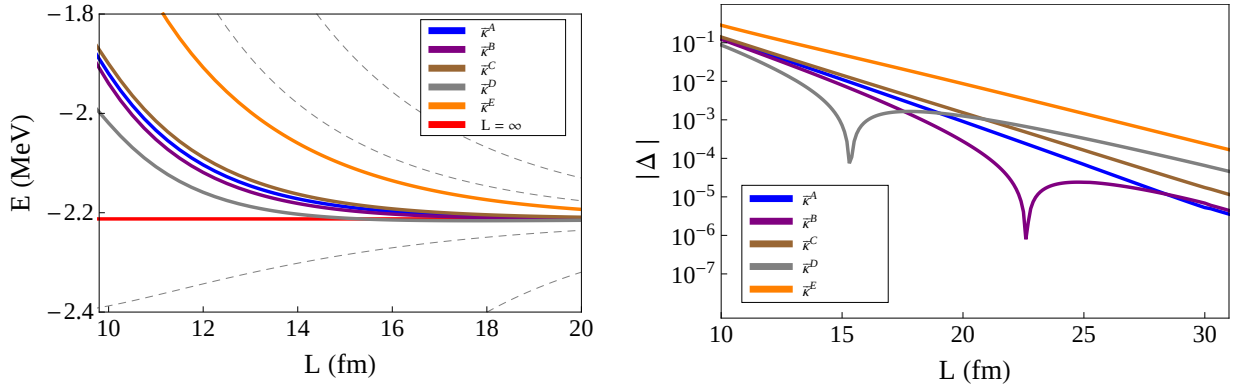

FIG. 4: The exponentially-improved estimates of the ground state energy in the deuteron channel from the $\overline{\kappa}^i$ relations given in eq. (11). The solid curves in the left panel shows the ground state energy associated with the $\overline{\kappa}^i$ relations, while the dashed (gray) lines show the ground state energies of the systems with a given momentum $\mathbf{P} = \frac{2\pi}{L}\mathbf{d}$, corresponding to the solid curves in fig. 3. The right panel shows the quantity $\Delta = (E(L) - E(\infty))/E(\infty)$ associated with the $\overline{\kappa}^i$ relations.

subtle cancellation between different volume dependences in the range of volumes that are shown in fig. 4.

IV. VOLUME-IMPROVED FITTING

While it is important to form the exponentially volume-improved combinations of binding momenta, it may not be the method that is actually implemented in the analysis of the results of LQCD calculations. The existence of the relations shows that the volume modifications in a prediction of the deuteron binding energy from one ensemble of gauge-field configurations can be exponentially reduced (in the NR-limit) with minimal additional computational resources. However, this reduction can also be accomplished simply by fitting the appropriate volume dependences to the results of the LQCD calculations for a range of $\mathbf{d}$. From eq. (9), the binding momentum for any given $\mathbf{d}$ is

$$\kappa^{(\mathbf{d})} \;=\; \kappa_0 \;+\; \frac{Z_\psi^2}{L}\; F^{(\mathbf{d})}(\kappa_0 L) \;+\; \mathcal{O}\left(e^{-2\kappa_0 L}/L\right) \quad , \tag{12}$$

with the coefficients and kinematic factors in $F^{(\mathbf{d})}(\kappa_0 L)$ determined by the lattice calculation. Therefore, up to $\mathcal{O}\left(e^{-2\kappa_0 L}/L\right)$, the two free-parameters that remain to be determined are κ_0 and Z_ψ which can be accomplished with a χ^2-minimization. In the case of having $\kappa^{(\mathbf{d})}$ for only two $\mathbf{d}$'s, κ_0 and Z_ψ can be solved for within the uncertainties of the LQCD calculations [3].

V. CONCLUSIONS

As recently stressed by Bour *et al*, the binding energy of a bound state depends upon its total momentum when subject to periodic boundary conditions in the spatial directions. Through the momentum modes excluded by the boundary conditions, these volume modifications of the binding energy depend upon the ratio of the spatial extent of the volume to the Lorentz-contracted size of the bound state, and also upon the masses of the constituents. We have extended the work of Bour *et al* from nonrelativistic quantum mechanics to quantum field theory and have pointed out that these features can be utilized in Lattice QCD calculations

[3] The volume extrapolation performed in Ref.[4] to determine the H-dibaryon binding energy, used the ground state energy obtained in two different lattice volumes and iteratively solved for κ_0 and Z_ψ in $\kappa^{(0,0,0)}$.

of hadronic bound states to (approximately exponentially) reduce the volume modifications of predicted binding energies. The standard Lattice QCD methodology that is used to determine the binding energy of a bound state is to measure the ground state energy of a system in a number of lattice volumes and then extrapolate to $L = \infty$ with a function of the form $\sim e^{-\kappa_0 L}/L + \mathcal{O}\left(e^{-\sqrt{2}\kappa_0 L}/L\right)$. Using combinations of boosted ground state energies, the volume dependence of the binding energy can be exponentially reduced in the nonrelativistic limit. For instance, the ground state energies of the lowest four boosted states in the lattice volume can be combined to reduce the volume modifications to the predicted binding energy to $\sim e^{-2\kappa_0 L}/L + \mathcal{O}\left(\eta^2 e^{-\kappa_0 L}/L\right)$ where $\eta \ll 1$.

In the specific case of the deuteron (neglecting its d-wave component), we have numerically explored what might be expected from future Lattice QCD calculations, and in particular, examined the volume dependence of combinations of boosted ground state energies. We find that the deuteron binding energy can be extracted to high precision in reasonably modest volumes, reducing the volume modifications by more than an order of magnitude over those of the state at rest for $L \gtrsim 10$ fm. It is also found that the volume modifications to the binding energy of the system with one unit of lattice momentum are significantly smaller than those of other low-momentum states, including the state at rest. It is clear that future Lattice QCD calculations that focus on extracting the properties and interactions of nuclei, including exotic systems such as the H-dibaryon, can greatly enhance the precision of their predicted binding energies by including systems with nonzero total momentum into their production.

We would like to thank William Detmold and Dean Lee for useful discussions. ZD and MJS were supported in part by the DOE grant DE-FG03-97ER4014. Not long after our preprint appeared on the arXive, work by Z. Fu [18] generalizing the Rummukainen and Gottlieb results to unequal mass systems in the context of πK scattering appeared.

Appendix A: Momentum Vectors Contributing to the Two-Particle Wavefunctions and the $Z_{LM}^{(\mathbf{d})}$ Functions

While eq. (1) has been derived in Refs. [12, 14, 15] for equal mass particles, in this appendix we outline the modifications to the derivation required for the case of unequal mass particles.

The derivation of Lüscher's formula for boosted systems is not repeated, but the momentum vectors that contribute to the summations defining the $Z_{LM}^{(\mathbf{d})}$ functions for a system comprised of particles of unequal mass are determined, along with the constraints on the two-particle wavefunctions.

Consider two particles of mass m_1 and m_2 with four-momenta P_1 and P_2. In the absence of external fields, the total momentum of the system, $P = P_1 + P_2$ is conserved, and the wavefunction of the system can be written as

$$\psi(x_1, x_2) \;=\; \psi(y, X) \;=\; e^{-iP\cdot X}\phi(y) \quad , \tag{A1}$$

where $y = x_1 - x_2$. The CoM coordinate, X, and the momentum conjugate to y, q, are such that the usual commutation relations are obtained when these quantities are promoted to quantum mechanical operators,

$$\left[\hat{\mathbf{X}}_i, \hat{\mathbf{P}}_j\right] = [\hat{\mathbf{y}}_i, \hat{\mathbf{q}}_j] = i\hbar\delta_{ij} \quad , \quad \left[\hat{\mathbf{X}}_i, \hat{\mathbf{q}}_j\right] = \left[\hat{\mathbf{y}}_i, \hat{\mathbf{P}}_j\right] = \left[\hat{\mathbf{X}}_i, \hat{\mathbf{y}}_j\right] = \left[\hat{\mathbf{q}}_i, \hat{\mathbf{P}}_j\right] = 0 \quad , \tag{A2}$$

from which it can be concluded that

$$P \;=\; P_1 + P_2 \;,\; y \;=\; x_1 - x_2 \;,\; X \;=\; \alpha x_1 + (1-\alpha)x_2 \;,\; q \;=\; (1-\alpha)P_1 - \alpha P_2 \;, \tag{A3}$$

where α is to be determined.

For particles with the same time-coordinate (i.e. on the same time-slice), $y_0 = 0$, in the rest frame of the cubic volume (the "laboratory frame"), the wavefunction in eq. (A1) can be written as $\psi_L(0, \mathbf{y}, T, \mathbf{X}) \;=\; e^{-i(ET - \mathbf{P}\cdot\mathbf{X})}\phi_L(0, \mathbf{y})$. In the CoM frame, the wavefunction takes the form $\psi_{CoM}(\mathbf{y}^*, T^*) = e^{-iE^*T^*}\phi_{CoM}(\mathbf{y}^*)$, and is, by construction, independent of the relative time coordinate. It is then the case that $\phi_L(0, \mathbf{y}) = \phi_{CoM}(\mathbf{y}^*) \;= \phi_{CoM}(\hat{\gamma}\mathbf{y})$. Further, as $\psi_{CoM}(\mathbf{y}^*, T^*)$ is independent of the relative time-coordinate, $\hat{P}^\mu \hat{q}_\mu \psi_{CoM}(\mathbf{y}^*, T^*) = 0$, and hence $q_0^* = 0$, from which it follows that

$$\alpha \;=\; \frac{1}{2}\left[\; 1 \;+\; \frac{m_1^2 - m_2^2}{E^{*2}} \;\right] \;, \tag{A4}$$

for a CoM energy of E^*, as given in eq. (3).

The periodic boundary conditions imposed on the wavefunction in each spatial direction requires that $\psi_L(0, \mathbf{y}, T, \mathbf{X})$ is invariant under spatial translations $\mathbf{x}_1 \to \mathbf{x}_1 + \mathbf{b}L$ and $\mathbf{x}_2 \to \mathbf{x}_2 + \mathbf{c}L$, where $\mathbf{b}$ and $\mathbf{c}$ are triplets of integers. For a total momentum of $\mathbf{P} = \frac{2\pi}{L}\mathbf{d}$, this invariance leads to

$$\phi_{\mathrm{L}}(\mathbf{y}) \;=\; e^{i2\pi\boldsymbol{\alpha}\mathbf{d}\cdot\mathbf{n}}\phi_{\mathrm{L}}(\mathbf{y} + \mathbf{n}L) \quad , \tag{A5}$$

where $\mathbf{n} = \mathbf{b} - \mathbf{c}$ is a triplet of integers, and it then follows that

$$\phi_{\rm CoM}(\mathbf{y}^*) \;=\; e^{i2\pi\alpha\mathbf{d}\cdot\mathbf{n}}\phi_{\rm CoM}(\mathbf{y}^* + L\hat{\gamma}\mathbf{n}) \quad . \tag{A6}$$

Fourier transforming eq. (A6) leads to a constraint on the allowed three-momenta in the CoM frame,

$$\mathbf{q} \;=\; \frac{2\pi}{L}\;\hat{\gamma}^{-1}\,(\mathbf{n}' - \alpha\mathbf{d}) \quad , \tag{A7}$$

where $\mathbf{n}'$ is a triplet of integers, as presented in eq. (2).

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[1] M. Luscher, Commun. Math. Phys. **104**, 177 (1986).

[2] S. R. Beane, P. F. Bedaque, A. Parreno and M. J. Savage, Phys. Lett. B **585**, 106 (2004) [arXiv:hep-lat/0312004].

[3] S. Sasaki and T. Yamazaki, Phys. Rev. D **74**, 114507 (2006) [arXiv:hep-lat/0610081].

[4] S. R. Beane *et al.* [NPLQCD Collaboration], Phys. Rev. Lett. **106**, 162001 (2011) [arXiv:1012.3812 [hep-lat]].

[5] S. R. Beane *et al.*, arXiv:1103.2821 [hep-lat].

[6] T. Inoue *et al.* [HAL QCD Collaboration], Phys. Rev. Lett. **106**, 162002 (2011) [arXiv:1012.5928 [hep-lat]].

[7] T. Yamazaki, Y. Kuramashi and A. Ukawa [PACS-CS Collaboration], Phys. Rev. D **81**, 111504 (2010) [arXiv:0912.1383 [hep-lat]].

[8] T. Yamazaki, Y. Kuramashi and A. Ukawa [PACS-CS Collaboration], arXiv:1105.1418 [hep-lat].

[9] S. Bour, S. Konig, D. Lee, H. W. Hammer and U. G. Meissner, arXiv:1107.1272 [nucl-th].

[10] M. Luscher, Commun. Math. Phys. **105**, 153 (1986).

[11] M. Luscher, Nucl. Phys. B **354**, 531 (1991).

[12] K. Rummukainen, S. A. Gottlieb, Nucl. Phys. **B450**, 397-436 (1995). [hep-lat/9503028].

[13] S. R. Beane, W. Detmold, K. Orginos and M. J. Savage, Prog. Part. Nucl. Phys. **66**, 1 (2011) [arXiv:1004.2935 [hep-lat]].

[14] C. h. Kim, C. T. Sachrajda and S. R. Sharpe, Nucl. Phys. B **727**, 218 (2005) [arXiv:hep-lat/0507006].

[15] N. H. Christ, C. Kim and T. Yamazaki, Phys. Rev. D **72**, 114506 (2005) [arXiv:hep-lat/0507009].

[16] P. F. Bedaque, I. Sato and A. Walker-Loud, Phys. Rev. D **73**, 074501 (2006) [arXiv:hep-lat/0601033].

[17] I. Sato and P. F. Bedaque, Phys. Rev. D **76**, 034502 (2007) [arXiv:hep-lat/0702021].

[18] Z. Fu, arXiv:1110.5975 [hep-lat].