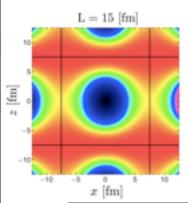
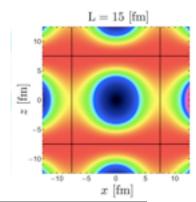


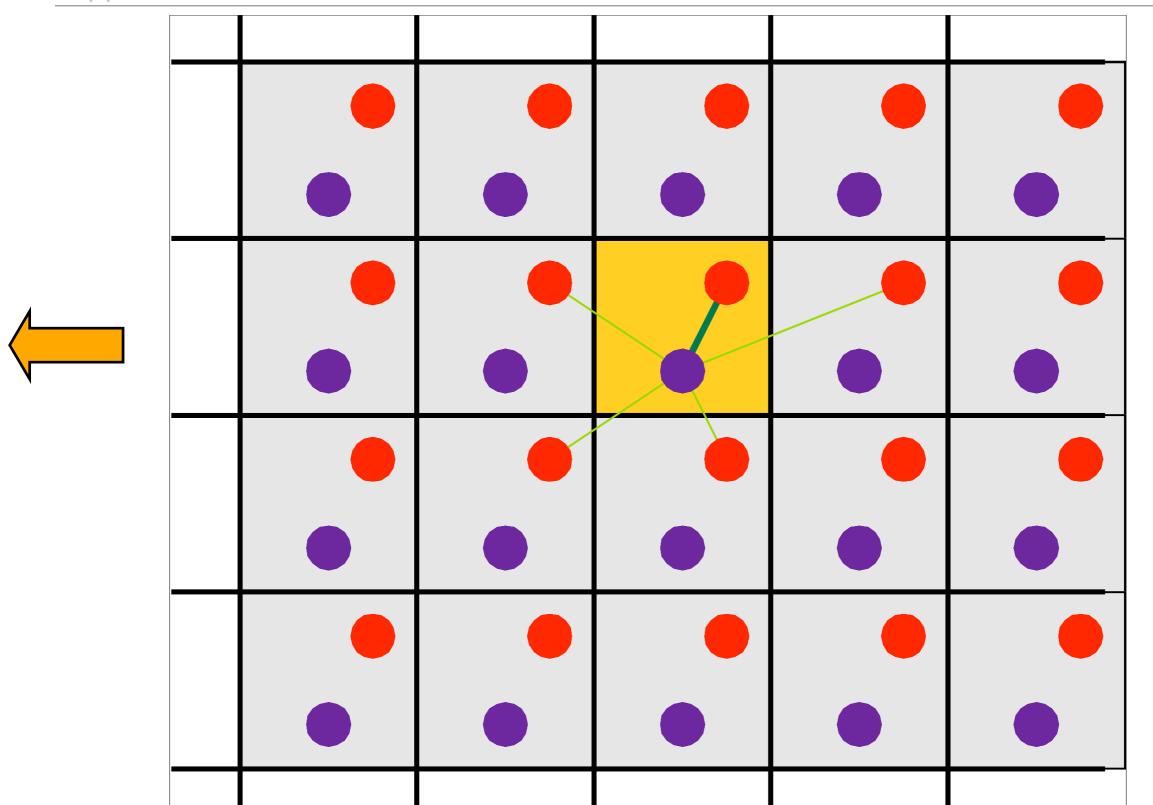
Twisted Boundary Conditions

Martin J. Savage Institute for Nuclear Theory October 2013

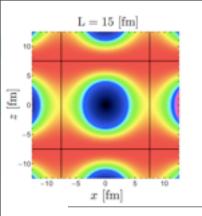


Periodic Boundary Conditions and Images

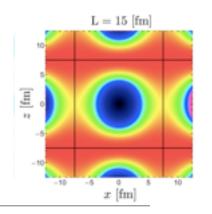








Two-Particle Energy Levels in Lattice QCD: Luscher

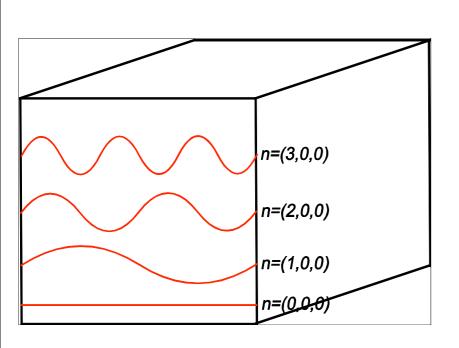


Below Inelastic Thresholds:

Measure on lattice

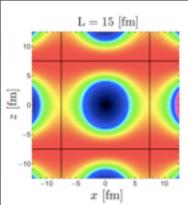
$$\delta E = 2\sqrt{p^2 + m^2} - 2m$$

$$p \cot \delta(p) = \frac{1}{\pi L} \mathbf{S} \left(\left(\frac{Lp}{2\pi} \right)^2 \right)$$

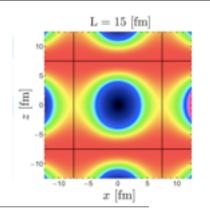


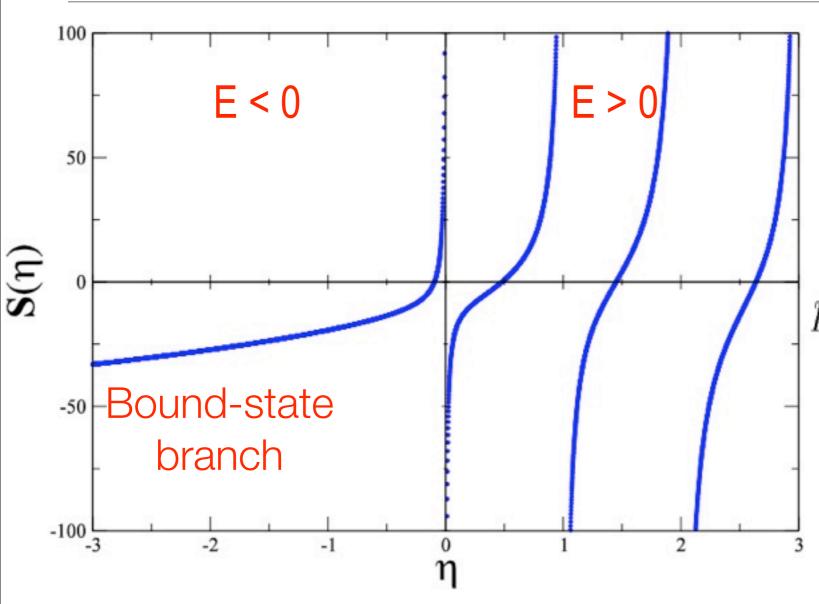
$$\mathbf{S}\left(\eta\right) \equiv \sum_{\mathbf{j}}^{\Lambda_{j}} \frac{1}{|\mathbf{j}|^{2} - \eta} - 4\pi\Lambda_{j}$$

Gives the scattering amplitude at δE



Luscher's Eigenvalue Relation





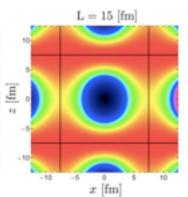
A₁⁺ Bound-state or Scattering state?

$$p \cot \delta(p) = \frac{1}{\pi L} \mathbf{S} \left(\left(\frac{Lp}{2\pi} \right)^2 \right)$$

$$\begin{aligned}
 V &= 0 \\
 S &= \infty
 \end{aligned}
 \quad \rightarrow \quad a = r = 0$$

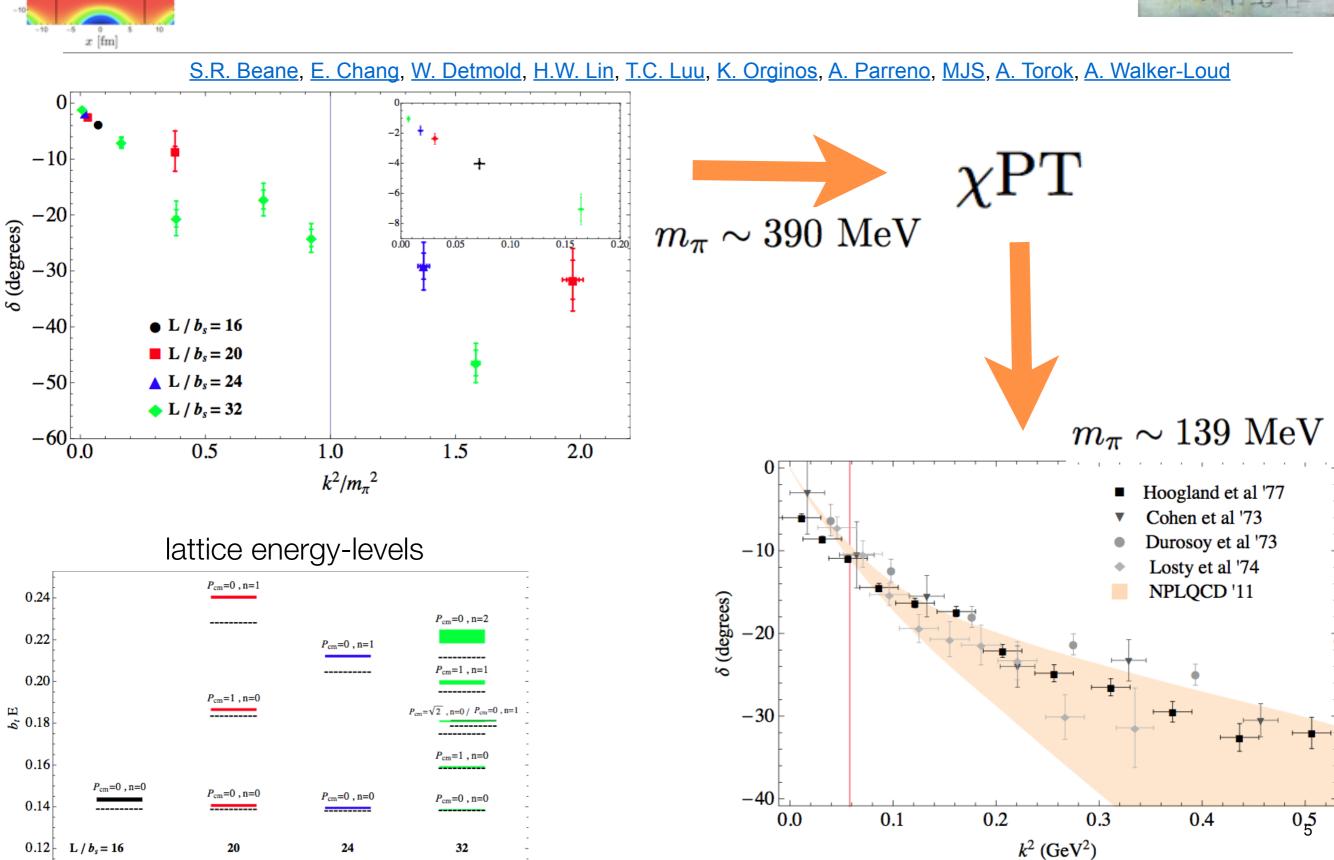
$$k = \frac{2\pi}{L}n$$

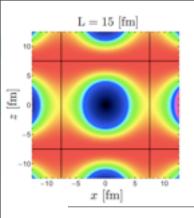
$$n = (nx, ny, nz)$$



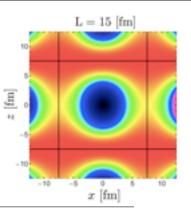
I=2 $\pi\pi$ Scattering Phase-Shift



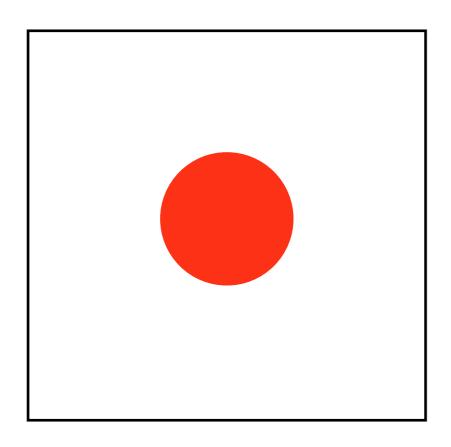


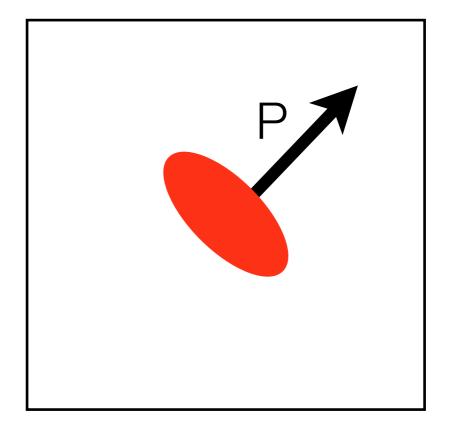


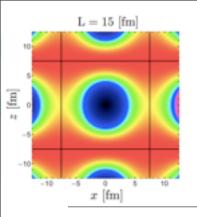
Bound-States in Motion



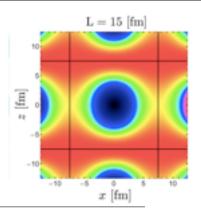
Consider an s-wave bound state:







Bound-States in Motion



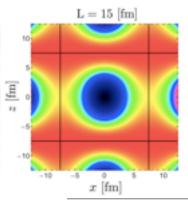
$$q^* \cot \delta(q^*) = \frac{2}{\gamma L \sqrt{\pi}} Z_{00}^{(\mathbf{d})}(1; \tilde{q}^{*2}, \tilde{\Delta}m_{12}^2)$$

$$\mathbf{P} = \frac{2\pi}{L} \, \mathbf{d}$$

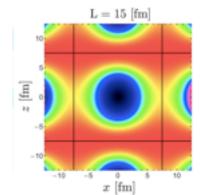
$$Z_{LM}^{(\mathbf{d})} = \sum_{\mathbf{r}} \frac{|\mathbf{r}|^L Y_{LM}(\Omega_{\mathbf{r}})}{|\mathbf{r}|^2 - \tilde{q}^{*2}}$$
, $\mathbf{r} = \frac{1}{\gamma} \left(\mathbf{n}_{\parallel} + \alpha \mathbf{d} \right) + \mathbf{n}_{\perp} = \hat{\gamma}^{-1} \left(\mathbf{n} + \alpha \mathbf{d} \right)$

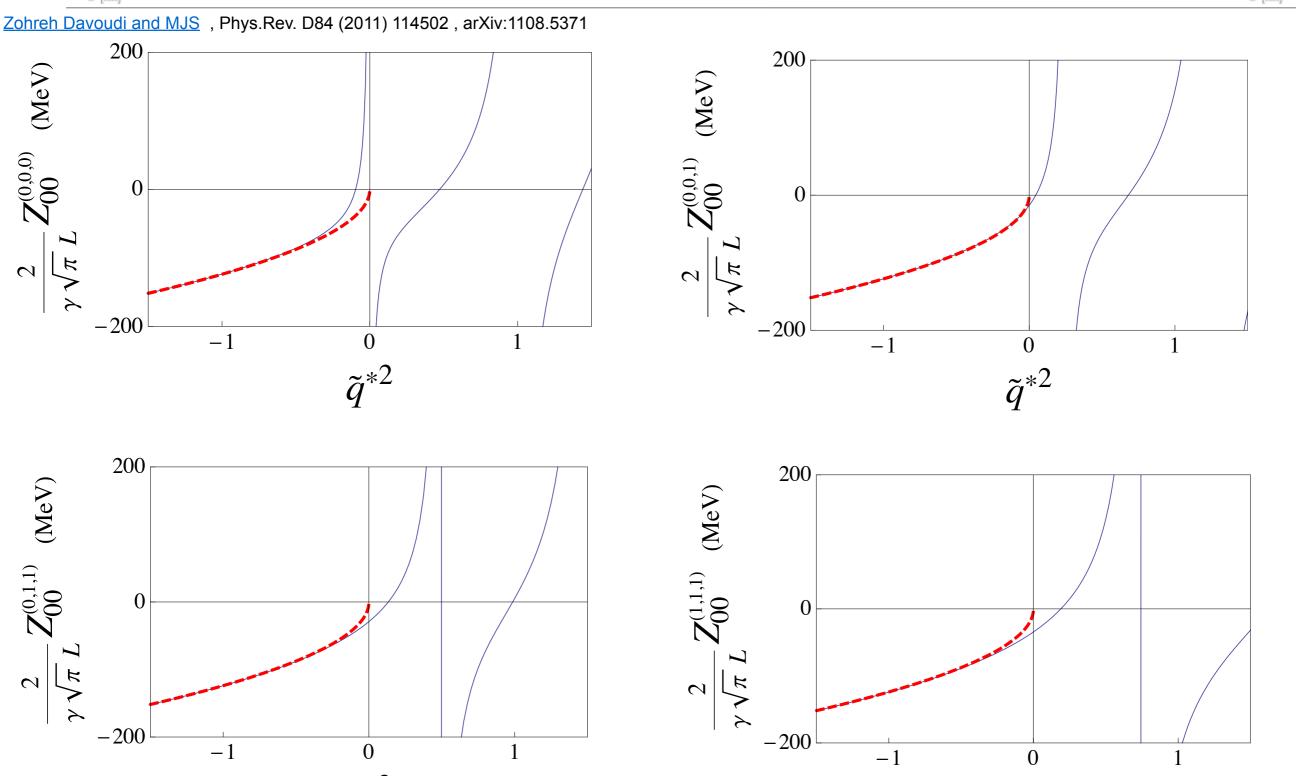
$$\alpha = \frac{1}{2} \left[1 + \frac{m_1^2 - m_2^2}{E^{*2}} \right]$$

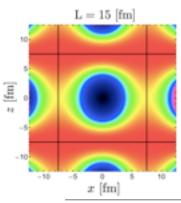
Gottlieb + Rummukainen and Kim, Sachrajda + Sharpe) equal mass



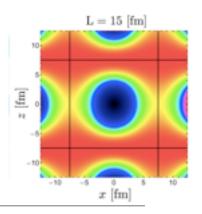
Bound-States in Motion Equal Masses



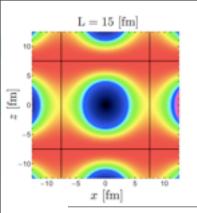




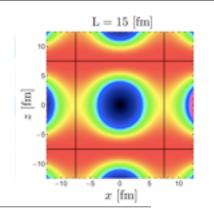
Bound-States in Motion Deuteron



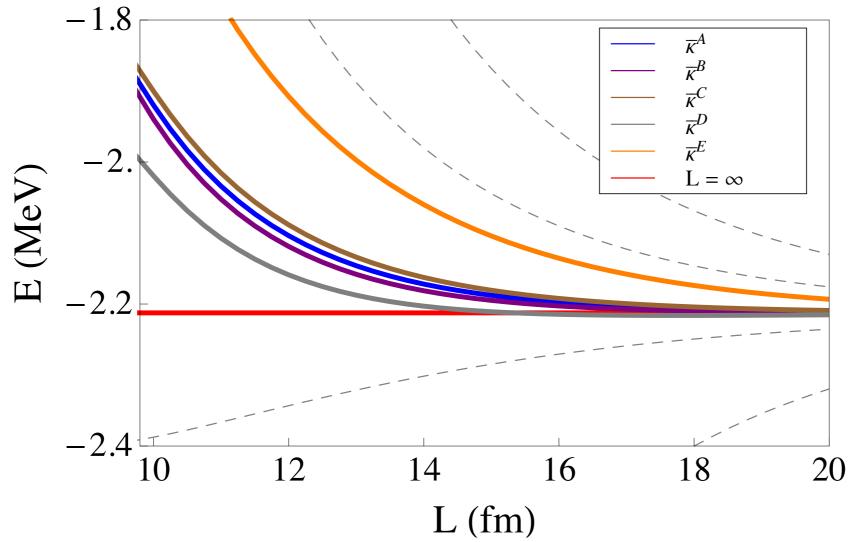
Zohreh Davoudi and MJS , Phys.Rev. D84 (2011) 114502 , arXiv:1108.5371



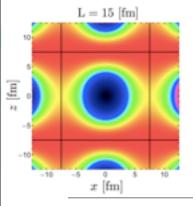
Bound-States in Motion Deuteron - Exponential Improvement



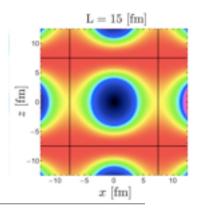
Zohreh Davoudi and MJS , Phys.Rev. D84 (2011) 114502 , arXiv:1108.5371



$$\overline{\kappa}^{A} = \frac{1}{8} \left(\kappa^{(0,0,0)} + 3\kappa^{(0,0,1)} + 3\kappa^{(0,1,1)} + \kappa^{(1,1,1)} \right)
= \kappa_{0} + \frac{3Z_{\psi}^{2}}{2L} \eta^{2} (1 + \kappa_{0}L) e^{-\kappa_{0}L} + \mathcal{O}\left(\eta^{4}e^{-\kappa_{0}L}L, \frac{e^{-2\kappa_{0}L}}{2L}\right) \qquad \eta = 0$$



Twisted BC's - History



January 28 2004

Aharonov-Bohm effect and nucleon-nucleon phase shifts on the lattice

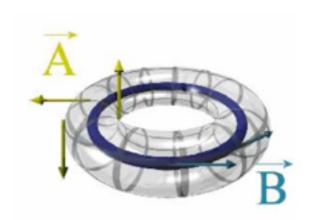
Paulo F. Bedaque*1 ¹Laurence-Berkeley Laboratory, Berkeley, CA 94720

We propose a method for the lattice QCD computation of nucleon-nucleon low-energy interactions. It consists in simulating QCD in the background of a "electromagnetic" field whose potential is nonvanishing, but whose field strength is zero. By tuning the background field, phase-shifts at any (but small) momenta can be determined by measuring the shift of the ground state energy. Lattice sizes as small as 5 Fermi can be sufficient for the calculation of phase shifts up to momenta of order of

One of the central goals of nuclear physics is to relate the successful phenomenological models developed throughout the years with the underlying fundamental theory of the strong interactions, QCD. Effective field theories are an important step in this direction, but they are inherently limited by the existence of low energy constants whose values are not determined by symmetries and have to be fit to experiment. The need is then obvious for a fully nonperturbative method that can determine the interaction between nucleons (or alternatively, the low energy constants of the effective theory) directly from QCD. At present, lattice QCD is the only such method.

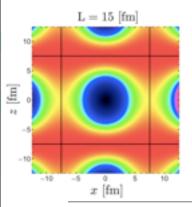
Most phenomenological models of nuclei are based on non-relativistic two(and three) nucleon potentials. However, since nucleons are not infinitely heavy, the inter-nucleon potential is not a well defined quantity that can be measured on the lattice, even in principle. Instead, the connection between QCD and nuclear physics should be established through observables like scattering amplitudes and phase shifts, etc.. That brings out a problem: lattice calculations are done in euclidean space and analytic continuation of the euclidean correlation functions at infinite volume to Minkowski space is, in practice, impossible. This observation, formalized in [1], seems to restrict lattice QCD to observables like masses, decays constants and amplitudes at kinematical thresholds. Phase shifts at some special FIG. 1: The lattice with periodic boundary conditions (and two dimensions suppressed) is represented by the surface of the values of the momenta can however be obtained by measuring the shifts in the low lying two-particle states due to the finite volume [2, 3, 4], as long as the lattice size L is larger than the pion Compton wavelength (up to corrections of order $e^{-m_{\pi}L}$). This can be intuitively understood by realizing that the baryon number two sector of QCD at momenta smaller than the pion mass reduces to a non relativistic quantum mechanical system with two nucleons interacting through contact interactions. At momenta Q much smaller than the $\sim 1/a$, where a is the nucleon-nucleon scattering length, this contact interaction is perturbative but it becomes strong at $Q \sim 1/a$. In particular, for lattices with size L much larger than the scattering length a the low lying states have typical momenta Q satisfying $Q \ll 1/a$, and Luscher derived the formula relating the shifts in the energy levels and a as an expansion in powers of a/L. This method has been used to obtain pion-pion scattering phase shifts in the two nucleon sector I am aware of only only one quenched calculation performed with a large pion mass 6

In the two-nucleon case the condition $L \gg a$ can hardly be satisfied since the scattering lengths between two

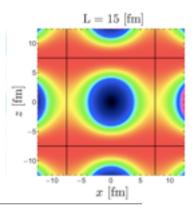


outer torus. The fictitious solenoid (inner ring) generates a magnetic vector potential \tilde{A} along direction z (wrapped around the torus). The magnetic field is confined inside the ring and vanishes at the surface of the torus, where the lattice is.

Paulo Bedaque, 2004



Twisted BC's - History



On the discretization of physical momenta in lattice QCD

G.M. de Divitiis a R. Petronzio N. Tantalo a

*University of Rome "Tor Vergata" and INFN sex. RomaII, Via della Ricerca Scientifica I., I-00133 Rome

Abstract

The adoption of two distinct boundary conditions for two fermions species on a finite lattice allows to deal with arbitrary relative momentum between the two particle species, in spite of the momentum quantization rule due to a limited physical box size. We test the physical significance of this topological momentum by checking in the continuum limit the validity of the expected energy-momentum dispersion relations.

1 Introduction

Among the restrictions of field theory formulations on a lattice, the finite volume momentum quantization represents a severe limitation in various phenomenological applications. For example, in a two body hadron decay where the energies of the decay products, related by 4-momentum conservation to the masses of the particles involved, cannot assume their physical values unLBNL-56738

Twisted valence quarks and hadron interactions on the lattice

Paulo F. Bedaque*

Laurence-Berkeley Laboratory, Berkeley, CA 94720, USA

Jiunn-Wei Chen!

Department of Physics and National Center for Theoretical Sciences at Taipei, National Taiwan University, Taipei, Taiwan 10617

Abstract

We consider QCD with valence and sea quarks obeying different boundary conditions. We point out that the energy of low lying two hadron states do not depend on the boundary condition of the sea quarks (up to exponentially small corrections). Thus, the advantages in using twisted boundary conditions on the lattice QCD extraction of nucleon-nucleon phase shifts can be gained without the need of new gauge configurations, even in fully unquenched calculations.

Twisted Boundary Conditions in Lattice Simulations

C.T. Sachrajda^a and G. Villadoro^b

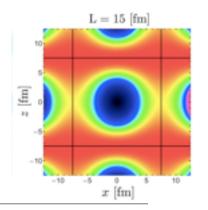
- ^a School of Physics and Astronomy, Univ. of Southampton, Southampton, SO17 1BJ, UK.
- ^b Dip. di Fisica, Univ. di Roma "La Sapienza" and INFN, Sezione di Roma, P.le A. Moro 2, I-00185 Rome, Italy.

Abstract

By imposing twisted boundary conditions on quark fields it is possible to access components of momenta other than integer multiples of 2r/L on a lattice with spatial volume L^2 . We use Chiral Perturbation Theory to study finite-volume effects with twisted boundary conditions for quantities without final-state interactions, such as meson masses, decay constants and semileptonic form factors, and confirm that they remain exponentially small with the volume. We show that this is also the case for partially twisted boundary conditions, in which (some of) the valence quarks satisfy twisted boundary conditions but the sea quarks satisfy periodic boundary conditions. This observation implies that it is not necessary to generate new gluon configurations for every choice of the twist angle, making the method much more practicable. For $K \to \pi\pi$ decays we show that the breaking of isospin symmetry by the twisted boundary conditions implies that the amplitudes cannot be determined in general (on this point we disagree with a recent claim).

Partially-Twisted BC's also have desirable properties

Twisted BC's - Pre-History



Twist-averaged Boundary Conditions in Continuum Quantum Monte Carlo

C. Lin, F.-H. Zong and D. M. Ceperley Dept. of Physics and NCSA, University of Illinois at Urbana-Champaign, Urbana, IL 61801

We develop and test Quantum Monte Carlo algorithms which use a "twist" or a phase in the wave function for fermions in periodic boundary conditions. For metallic systems, averaging over the twist results in faster convergence to the thermodynamic limit than periodic boundary conditions for properties involving the kinetic energy with the same computational complexity. We determine exponents for the rate of convergence to the thermodynamic limit for the components of the energy of coulomb systems. We show results with twist averaged variational Monte Carlo on free particles, the Stoner model and the electron gas using Hartree-Fock, Slater-Jastrow, three-body and backflow wavefunction. We also discuss the use of twist averaging in the grand canonical ensemble, and numerical methods to accomplish the twist averaging.

PACS Numbers: 02.70.-c, 82.20.Wt, 71.15.-m

22 Jan 200

[cond-mat.stat-mech]

arXiv:cond-mat/0101339v1

Almost all quantum Monte Carlo (QMC) calculations in periodic boundary conditions have assumed that phase of the wavefunction returns to the same value if a particle goes around the periodic boundaries and returns to its original position. However, with these boundary conditions, delocalized fermion systems converge slowly to the thermodynamic limit because of shell effects in the filling of single particle states. In this paper we explore an alternative boundary condition: one can allow particles to pick up a phase when they wrap around the periodic boundaries.

$$\Psi(\mathbf{r}_1 + L\hat{\mathbf{x}}, \mathbf{r}_2, \cdots) = e^{i\theta_x}\Psi(\mathbf{r}_1, \mathbf{r}_2, \cdots).$$
 (1)

The boundary condition $\theta = 0$ is called periodic boundary conditions (PBC), $\theta = \pi$ anti-periodic boundary conditions (ABC) and the general condition with $\theta \neq 0$, twisted boundary conditions (TBC).

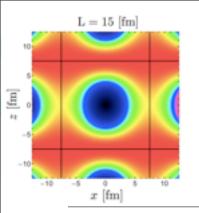
In periodic boundary conditions, the Hamiltonian is invariant with respect to translating any particle around the periodic boundaries. According to Bloch's theorem, this implies that any solution can be characterized by a given twist angle. The twist angle also has a physical origin: consider a toroidal geometry. One can either rotate the torus and go into rotating coordinates, or add a magnetic flux to the center of the torus. The physical properties will be unchanged. In both cases one can transform away the perturbation by applying TBC with the twist angle given by $\theta = mR^2\omega/h$ for rotation and $\theta = e\phi/(c\hbar)$ for magnetic flux. A torus is topologically equivalent to periodic boundary conditions, so that a non-zero twist will be allowed in periodic boundaries. The twist is a degree of freedom, or boundary condition, that can be varied to enable a finite system to approach the thermodynamic limit more quickly or to make decan be restricted to be in the range:

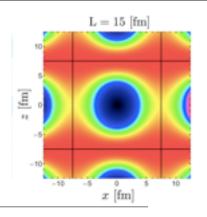
$$-\pi < \theta_i \le \pi$$
. (2)

For systems with a real potential (e.g. no magnetic field), one can further restrict the twist to be in the range $[0, \pi]$.

For a degenerate Fermi liquid, finite-size shell effects are much reduced if the twist angle is averaged over. We call this twist averaged boundary conditions (TABC) This is particularly important in computing properties that are sensitive to the single particle energies such as the kinetic energy and the magnetic susceptibility. By reducing shell effects, much more accurate estimations of the thermodynamic limit of these properties can be made. What makes this even more important is that the most accurate quantum methods have computational demands which increase rapidly with the number of fermions. Examples of such methods are exact diagonalization (exponential increase in CPU time with N), variational Monte Carlo (VMC) with wavefunctions having backflow and three-body terms (increases as N⁴), and transient-estimate and released-node Diffusion Monte Carlo methods (exponential increase with N). Methods which can extrapolate more rapidly to the thermodynamic limit are crucial in obtaining high accuracy. Twist averaging is especially advantageous for stochastic methods (i.e. QMC) because the averaging does not necessarily slow down the evaluation of averages, except for the necessity of doing complex rather than real arith-

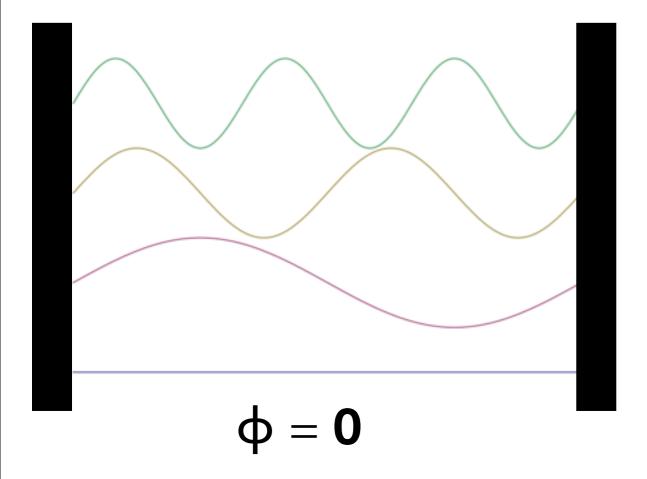
The use of twisted boundary conditions is commonplace for the solution of the band structure problem for a periodic solid. Band structure methods begin by assuming the wavefunction factors into single particle or-

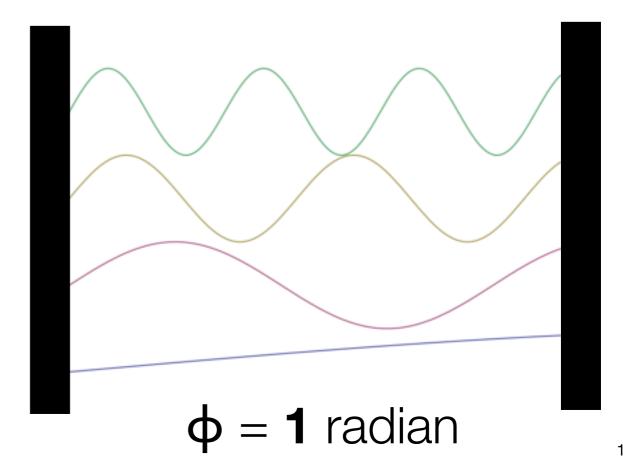




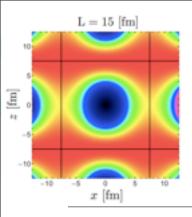
$$q_i(x+L,y+L,z+L) = e^{i\phi_x^i}e^{i\phi_y^i}e^{i\phi_z^i}q_i(x,y,z)$$

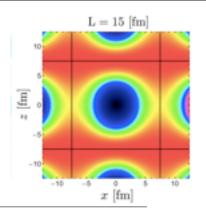
$$k L = 2 \pi n + \phi$$

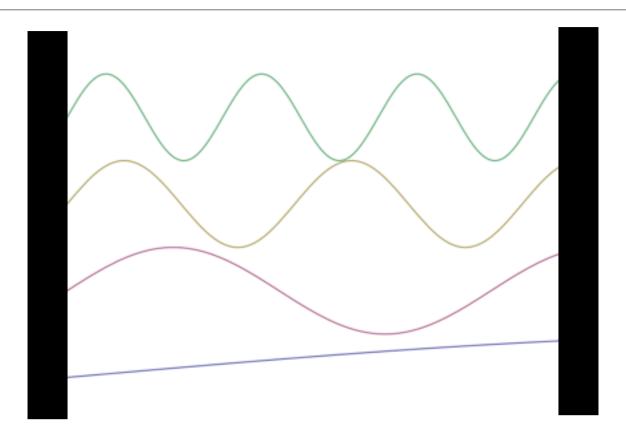




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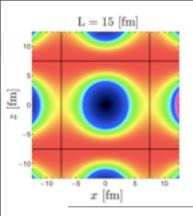


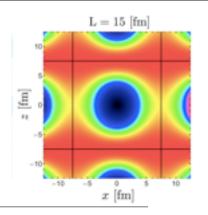




By choosing a particular ϕ can put levels in "desired place"

- dial kinematics



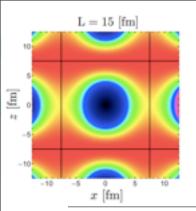


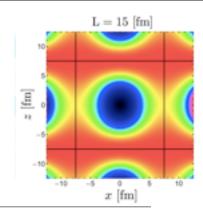
$$k L = 2 \pi n + \phi$$

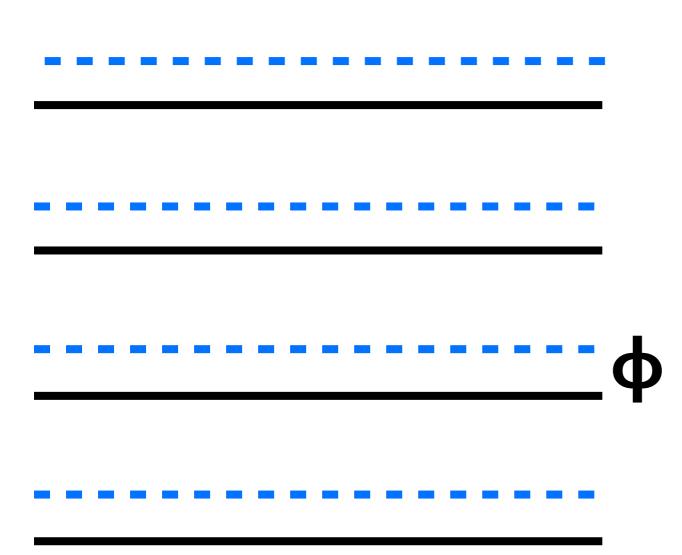
$$\int \frac{dk}{2\pi} f(k) \rightarrow \frac{1}{L} \sum_{n \in \mathbb{Z}_1} f(\frac{2\pi n + \phi}{L}) \qquad \text{• Volume Corrections present}$$

- - Multiple "runs" required to systematically reduce

$$\int \frac{dk}{2\pi} f(k) = \int \frac{d\phi}{2\pi} \frac{1}{L} \sum_{n \in \mathbb{Z}} f(\frac{2\pi n + \phi}{L}) \bullet \text{No Volume Corrections}$$

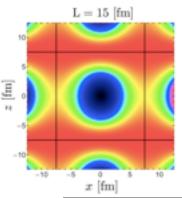






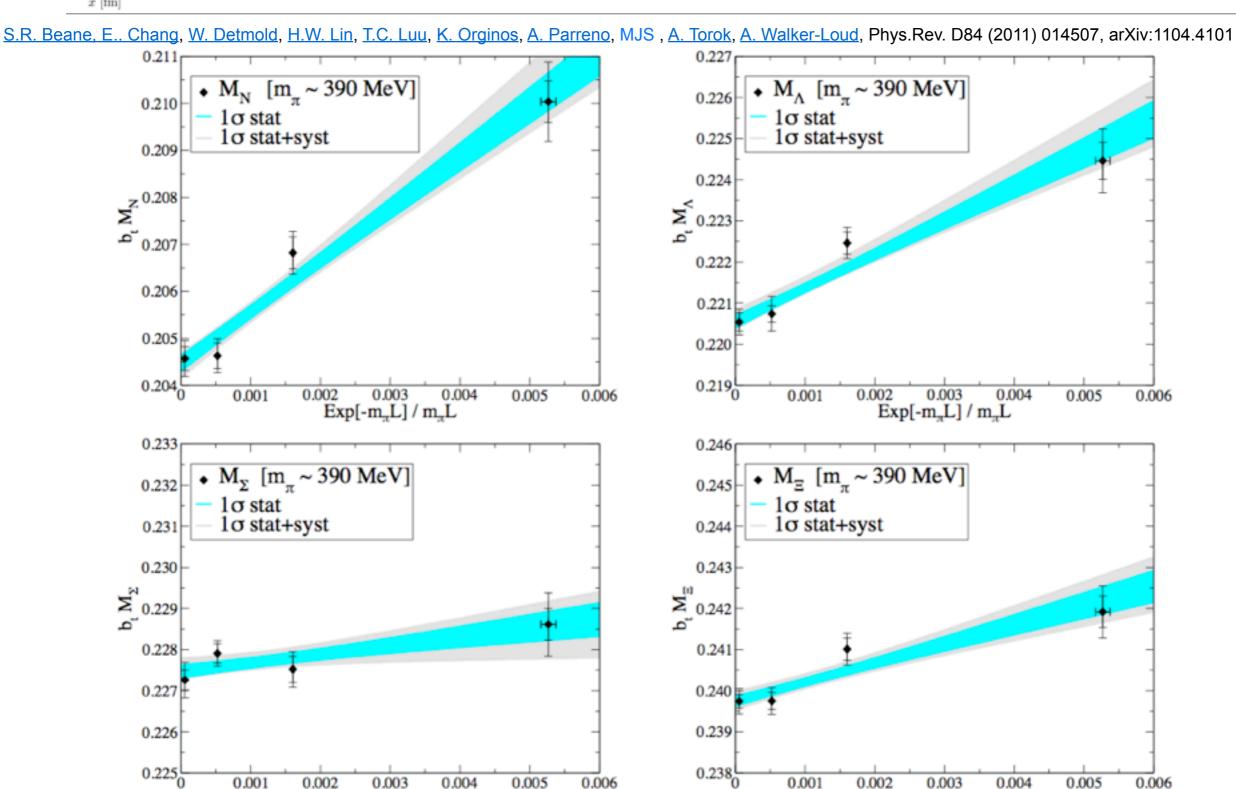
$$k L = 2 \pi n + \phi$$

Summing over ${f n}$ and integrating over ${f \varphi}$ is equivalent to integrating over ${f k}$



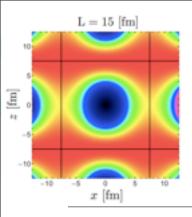
Nucleon Mass in FV Lattice QCD Calculations



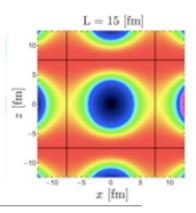


 $Exp[-m_{\pi}L]/m_{\pi}L$

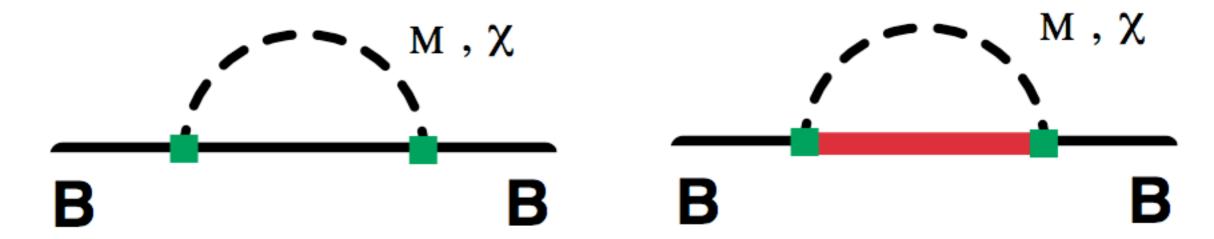
 $Exp[-m_{\pi}L]/m_{\pi}L$



Nucleon Mass in FV



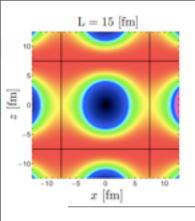
S. R. Beane, Phys.Rev. D70 (2004) 034507, hep-lat/0403015



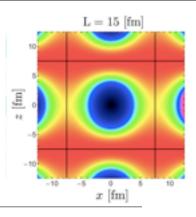
$$oldsymbol{\phi}^u = rac{1}{3}oldsymbol{ heta} \;,\;\; oldsymbol{\phi}^d = -rac{2}{3}oldsymbol{ heta} \ oldsymbol{\phi}^{\pi^+} = oldsymbol{ heta} \;,\;\; oldsymbol{\phi}^{\pi^-} = -oldsymbol{ heta} \;\;,\;\; oldsymbol{\phi}^{\pi^0,\eta^0} = 0 \ oldsymbol{\phi}^n = -oldsymbol{ heta} \;\;,\;\; oldsymbol{\phi}^p = 0$$

$$I \sim \sum_{\mathbf{k}} \frac{m_{\pi}^2}{|\mathbf{k}|^2 + m_{\pi}^2} \sim -\frac{g_A^2 m_{\pi}^2}{8\pi f^2} \left[\frac{3}{2} m_{\pi} - \frac{1}{L} \sum_{\mathbf{p} \neq \mathbf{0}} \frac{1}{|\mathbf{p}|} e^{-|\mathbf{p}| m_{\pi} L} \left(e^{-i\mathbf{p} \cdot \phi^{\pi^+}} + \frac{1}{2} \right) \right]$$

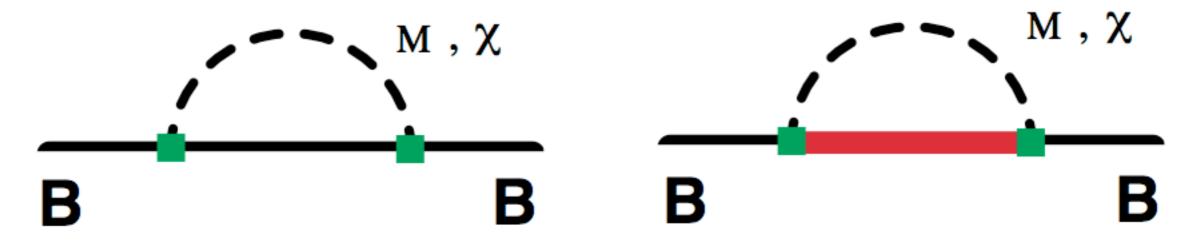
FV effects



Nucleon Mass in FV



Raul A. Briceno, Zohreh Davoudi, Thomas Luu, MJS

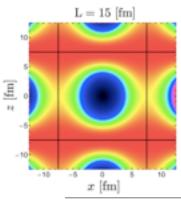


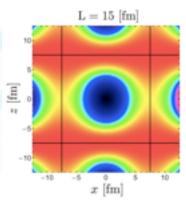
$$\frac{3}{2} \rightarrow \langle e^{-i\mathbf{p}\cdot\phi^{\pi^+}} + \frac{1}{2} \rangle_{\phi} = \frac{1}{2}$$

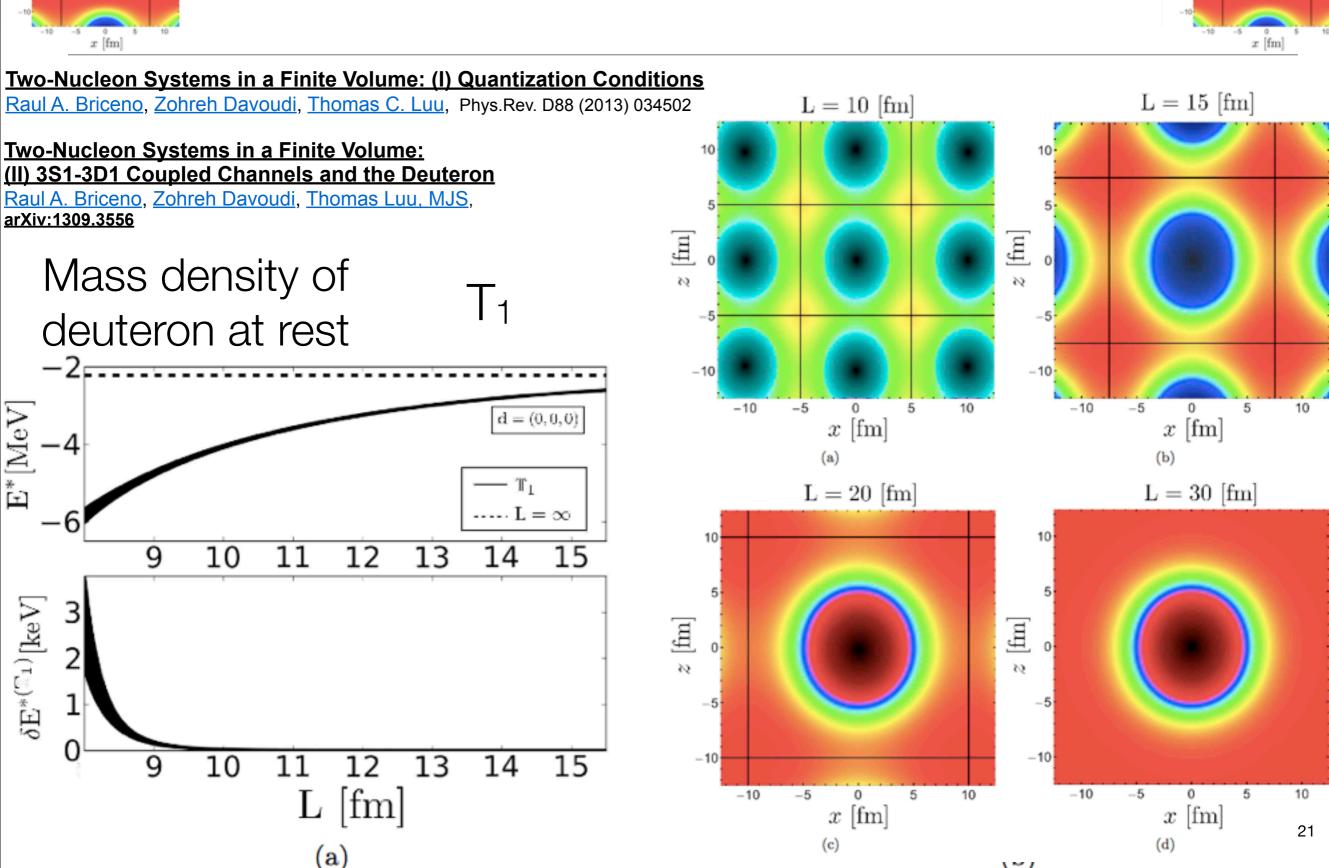
Twist Averaging

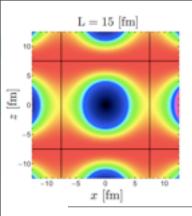
or choose twists to eliminate/suppress the leading FV contribution

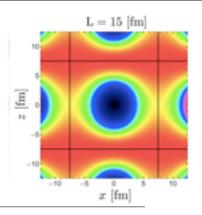
'Nice' linear example









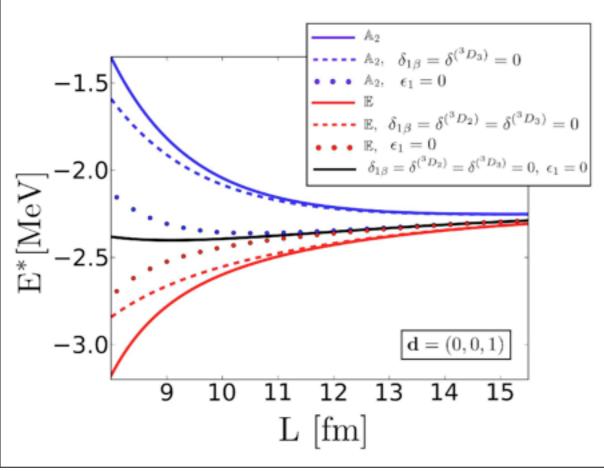


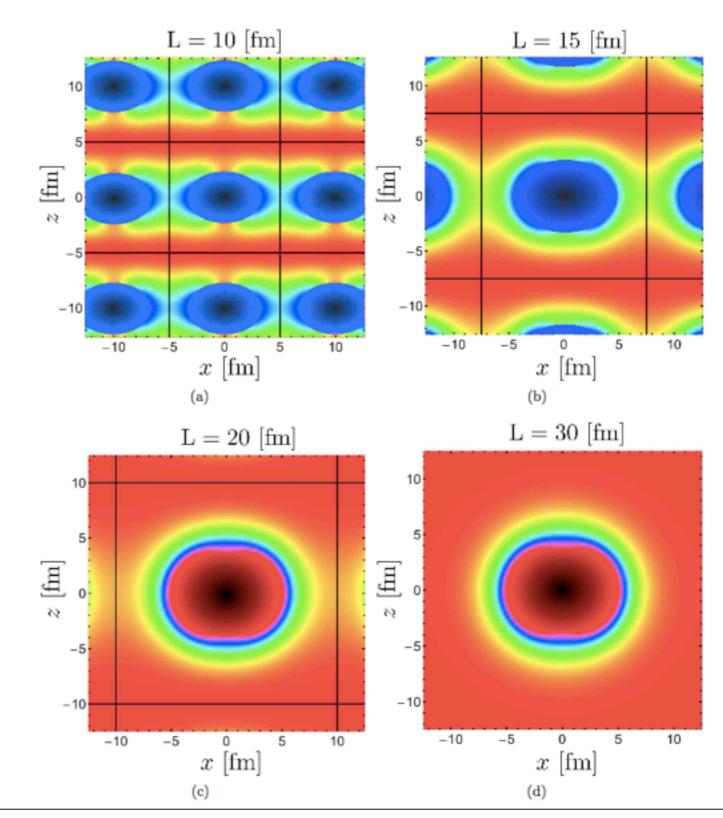
Two-Nucleon Systems in a Finite Volume: (II) 3S1-3D1 Coupled Channels and the Deuteron

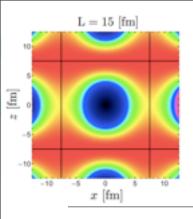
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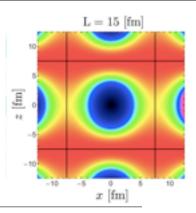
arXiv:1309.3556

Mass density of boosted deuteron d=(0,0,1)

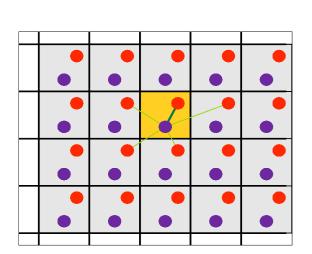








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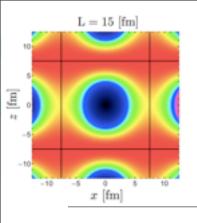
$$\psi(x_1, x_2) = \psi_{\text{Lab}}(t, \mathbf{y}, T, X) = e^{-iET} e^{i\mathbf{P}\cdot\mathbf{X}} \Phi_L(0, \mathbf{y})$$
 $P = p_1 + p_2 , q = (1 - \alpha)p_1 + \alpha p_2$
 $\mathbf{X} = \alpha \mathbf{x}_1 + (1 - \alpha)\mathbf{x}_2 , \mathbf{y} = \mathbf{x}_1 - \mathbf{x}_2$
 $\alpha = \frac{1}{2} \left(1 + \frac{m_1^2 - m_2^2}{E^{*2}}\right)$

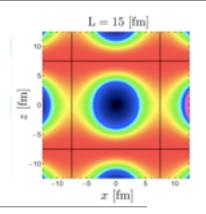
$$\mathbf{x}_1 \to \mathbf{x}_1' = \mathbf{x}_1 + \mathbf{b}L \text{ and } \mathbf{x}_2 \to \mathbf{x}_2' = \mathbf{x}_2 + \mathbf{c}L$$

$$\psi_{\text{Lab}}(0, \mathbf{y}', T, X') = e^{i(\mathbf{b} \cdot \phi_1 + \mathbf{c} \cdot \phi_2)} \psi_{\text{Lab}}(0, \mathbf{y}, T, X)$$

$$e^{i2\pi\alpha\mathbf{d} \cdot \mathbf{n}} e^{i(2\alpha - 1)\mathbf{n} \cdot (\phi_1 + \phi_2)/2} e^{i\mathbf{n} \cdot (\phi_2 - \phi_1)/2} \Phi_L(\mathbf{y} + \mathbf{n}L) = \Phi_L(\mathbf{y})$$

$$\mathbf{k} = \frac{1}{L} \hat{\gamma}^{-1} \left(2\pi \mathbf{n} - 2\pi \alpha \mathbf{d} - \frac{1}{2} (2\alpha - 1)(\phi_1 + \phi_2) - \frac{1}{2} (\phi_2 - \phi_1) \right)$$





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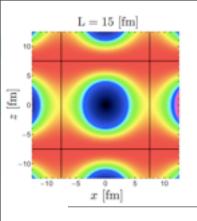
$$\mathbf{k} = \frac{1}{L} \hat{\gamma}^{-1} \left(2\pi \mathbf{n} - 2\pi \alpha \mathbf{d} - \frac{1}{2} (2\alpha - 1)(\phi_1 + \phi_2) - \frac{1}{2} (\phi_2 - \phi_1) \right)$$

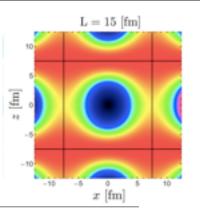
$$\mathbf{m}_1 = \mathbf{m}_2$$
, $\mathbf{\alpha} = 0$ $\mathbf{k} = \frac{1}{L} \hat{\gamma}^{-1} \left(2\pi \mathbf{n} - \pi \mathbf{d} - \frac{1}{2} (\phi_2 - \phi_1) \right)$

$$m_1=m_2$$
 , $\alpha=0$, $\varphi_1=\varphi_2$

$$\mathbf{k} \,=\, rac{2\pi}{L}\; \hat{\gamma}^{-1} \left(\; \mathbf{n} \;-\; rac{1}{2} \mathbf{d}\;
ight)$$

If both particles have the same twist then no change in relative momenta





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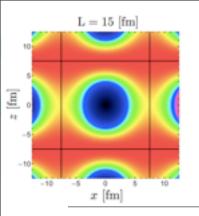
$$\begin{aligned} p\cot\delta(p)\big|_{p=i\kappa} \; + \; \kappa \; &= \; \frac{1}{\mathcal{L}} \; \sum_{\mathbf{n}\neq\mathbf{0}} \; \frac{1}{|\hat{\gamma}\mathbf{n}|} \; e^{i2\pi\alpha\mathbf{n}\cdot\mathbf{d}} \; e^{i(2\alpha-1)\mathbf{n}\cdot(\phi_1+\phi_2)/2} \; e^{i\mathbf{n}\cdot(\phi_1-\phi_2)/2} \; e^{-|\hat{\gamma}\mathbf{n}|\kappa\mathcal{L}} \\ \boldsymbol{\phi}^u \; &= \; \boldsymbol{\theta} \; \; , \quad \boldsymbol{\phi}^d \; = \; -\boldsymbol{\theta} \\ \boldsymbol{\phi}^{\pi^+} \; &= \; 2\boldsymbol{\theta} \; \; , \quad \boldsymbol{\phi}^{\pi^-} \; = \; -2\boldsymbol{\theta} \; \; , \quad \boldsymbol{\phi}^{\pi^0,\eta^0} \; = \; 0 \\ \boldsymbol{\phi}^n \; &= \; -\boldsymbol{\theta} \; \; , \quad \boldsymbol{\phi}^p \; = \; \boldsymbol{\theta} \end{aligned}$$

Transcendental equation provides the two-body binding energy

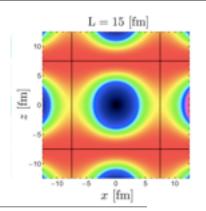
Twist averaging

 $\boldsymbol{\phi}^{np} = 0 .$

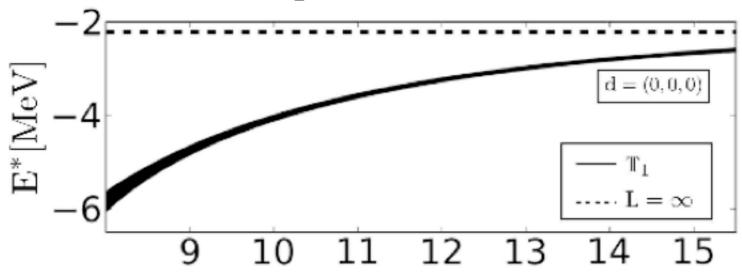
- will not give the infinite-volume binding
- much closer

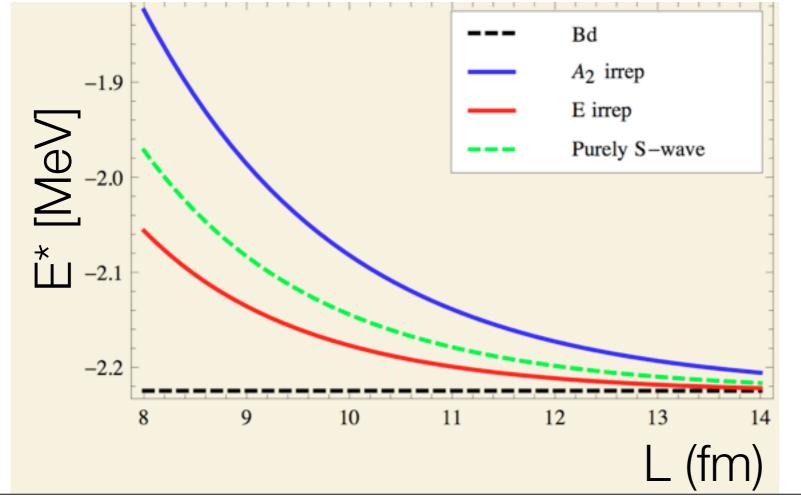


Two-Body Bound-States Twisted Deuteron

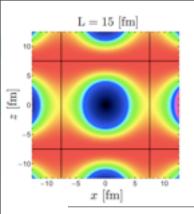


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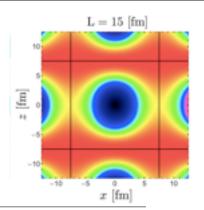




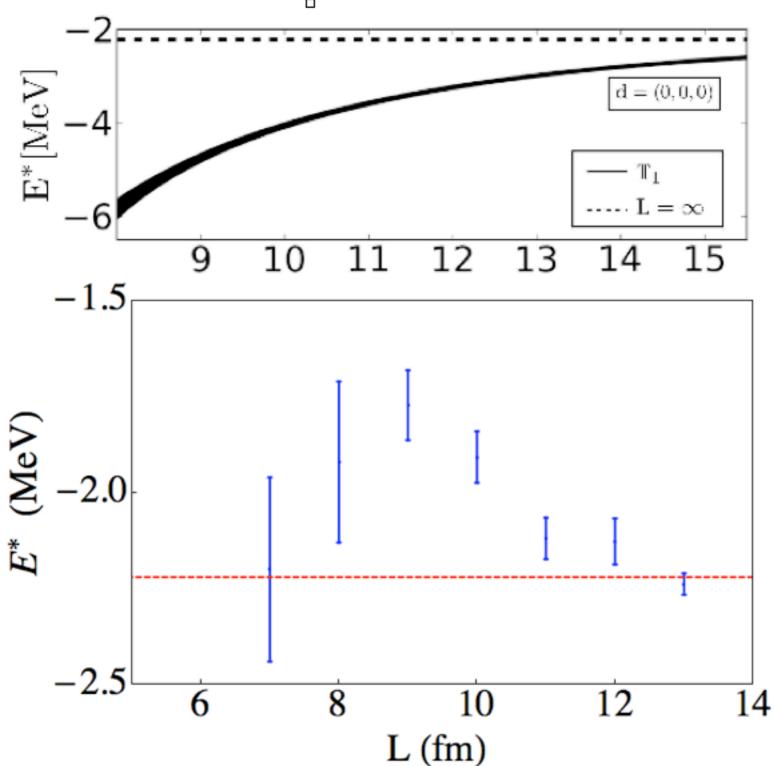
$$\phi = \left(\frac{\pi}{2}, \frac{\pi}{2}, \frac{\pi}{2}\right)$$



Two-Body Bound-States Twisted-Averaged Deuteron

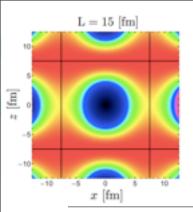


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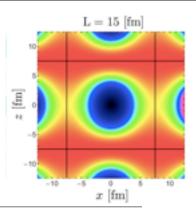


$$\langle E^* \rangle_{\theta}$$

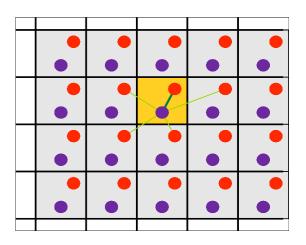
100 random twists



Summary



- Periodic BC's have FV effects
 - can be large
 - can require multiple "runs" to systematically reduce



- Free to include arbitrary twist to BC's to modify FV effects
- \bullet Theoretical guidance to choose ϕ to minimize FV effects
- Twist averaging can eliminate FV effects in some cases
 - linear quantities
 - exponentially reduce FV effects in deuteron Raul A. Briceno, Zohreh Davoudi, Thomas Luu, MJS

