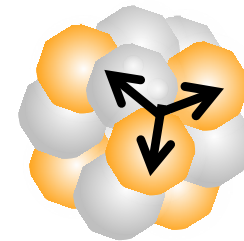
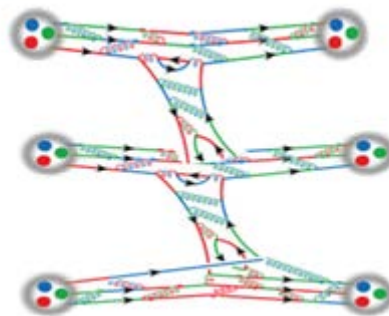
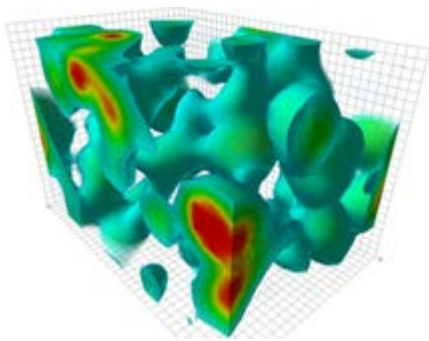


# Three-Nucleon Forces from Lattice QCD

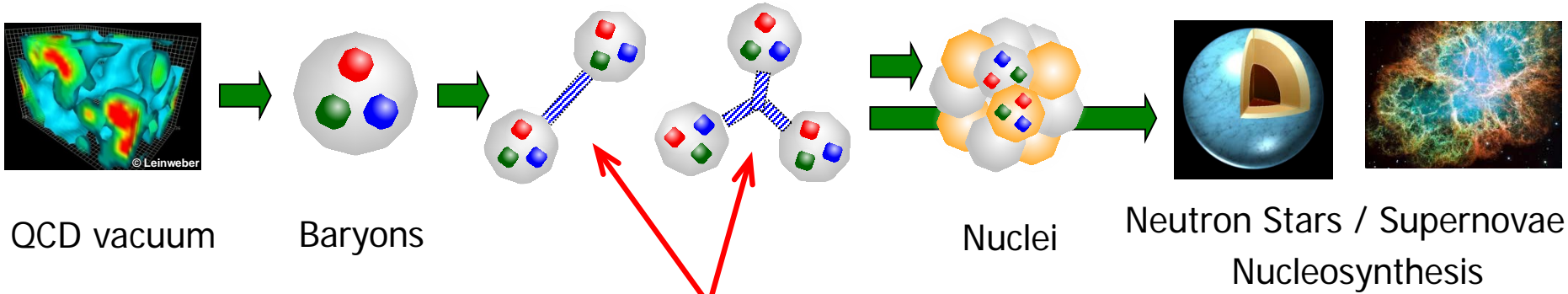
**Takumi Doi**

(RIKEN Nishina Center / iTHEMS)

for HAL QCD Collaboration



# The Odyssey from Quarks to Universe

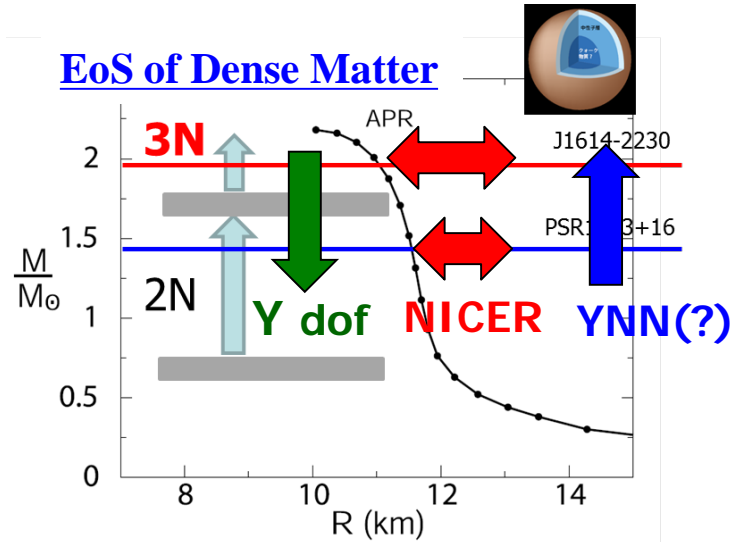
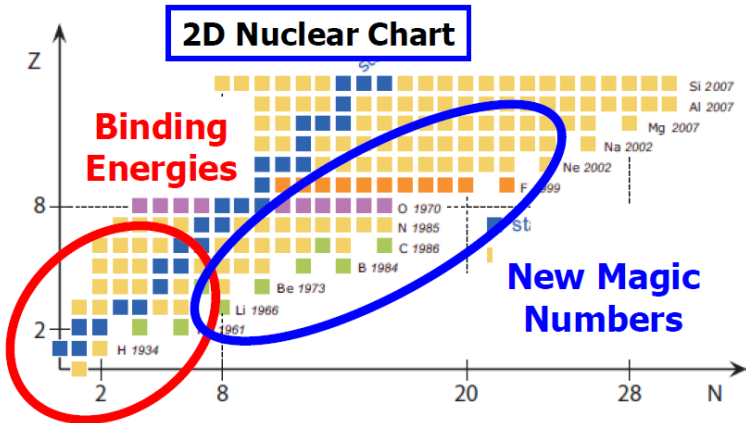


QCD

1st-principle Lattice QCD

Baryon Forces

ab-initio nuclear calc.



# [HAL QCD method]

- Nambu-Bethe-Salpeter (NBS) wave function

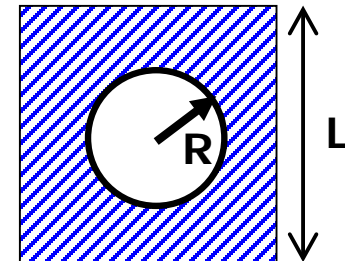
$$\psi(\vec{r}) = \langle 0 | N(\vec{r})N(\vec{0}) | N(\vec{k})N(-\vec{k}); W \rangle$$

$$(\nabla^2 + k^2)\psi(\vec{r}) = 0, \quad r > R$$

- phase shift at asymptotic region

$$\psi(r) \simeq A \frac{\sin(kr - l\pi/2 + \delta(k))}{kr}$$

**Phase shift in 2-body scattering**



M.Luscher, NPB354(1991)531

C.-J.Lin et al., NPB619(2001)467

N.Ishizuka, PoS LAT2009 (2009) 119

CP-PACS Coll., PRD71(2005)094504

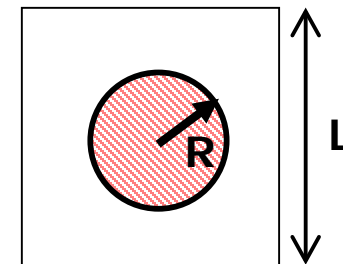
- Consider the wave function at “interacting region”

$$(\nabla^2 + k^2)\psi(\mathbf{r}) = m \int d\mathbf{r}' U(\mathbf{r}, \mathbf{r}') \psi(\mathbf{r}'), \quad r < R$$

- $U(\mathbf{r}, \mathbf{r}')$ : faithful to the phase shift by construction

- $U(\mathbf{r}, \mathbf{r}')$ : **E-independent**, while **non-local** in general

- Non-locality  $\rightarrow$  derivative expansion



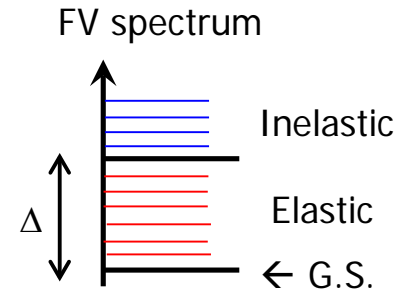
Aoki-Hatsuda-Ishii PTP123(2010)89

# [Time-dependent HAL QCD method]

*E-indep of potential  $U(\mathbf{r}, \mathbf{r}')$   $\rightarrow$  (excited) scatt states share the same  $U(\mathbf{r}, \mathbf{r}')$*

$$\int d\mathbf{r}' U(\mathbf{r}, \mathbf{r}') R(\mathbf{r}', t) = \left( -\frac{\partial}{\partial t} + \frac{1}{4m} \frac{\partial^2}{\partial t^2} - H_0 \right) R(\mathbf{r}, t)$$

	Ground state	Excited (elastic)	Excited (inelastic)
HAL method	Signal	Signal	Noise
Direct method	Signal	Noise	Noise

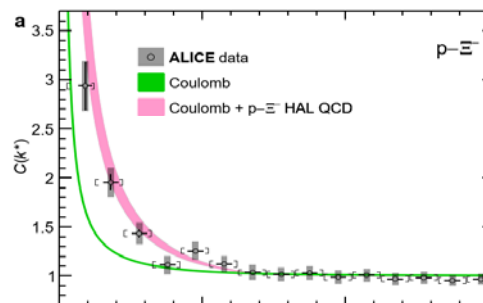
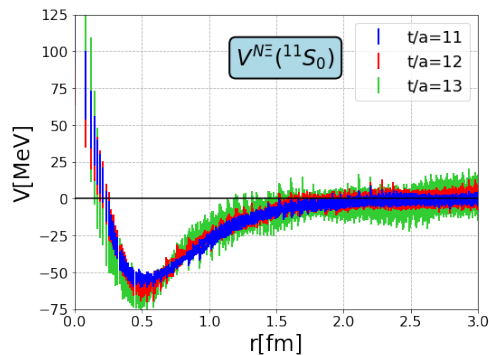


**HAL method  $\rightarrow$  Exponentially better S/N**

Direct method = Plateau fit w/ GS saturation  
+ Luscher's formula

## Two-Baryon Forces:

**near physical point simulation successfully performed!**



S. Gongyo et al.. (HAL) PRL120(2018)212001  
T. Iritani et al. (HAL) PLB792(2019)284  
K. Sasaki et al. (HAL) NPA998(2020)121737  
Y. Lyu, H. Tong et al. PRL127(2021)072003

Calc of charmed int:  
 $\rightarrow$  Y. Lyu's talk

**and confirmed by ALICE**

# Extension to multi-particle systems ( $n \geq 3$ )

S.Aoki et al. (HAL Coll.), PRD88(2013)014036

- Unitarity of S-matrix

$$T^\dagger - T = iT^\dagger T$$

Hyper-spherical func in  $D=3(n-1)$  dim

$$T([\mathbf{q}^A]_n, [\mathbf{q}^B]_n) = \sum_{[L],[K]} T_{[L][K]}(Q_A, Q_B) Y_{[L]}(\Omega_{Q_A}) \overline{Y_{[K]}(\Omega_{Q_B})}$$

$$[L] = L, M_1, M_2, \dots$$

diagonalization

$$T_{[L][K]}(Q, Q) = \sum_{[N]} U_{[L][N]}(Q) T_{[N]}(Q) U_{[N][K]}^\dagger(Q) \quad (Q = Q_A = Q_B)$$

$$T_{[L]}(Q) = -\frac{2n^{3/2}}{mQ^{3n-5}} \boxed{e^{i\delta_{[L]}(Q)} \sin \delta_{[L]}(Q)}$$

c.f. R.B. Newton (1974) for  $n = 3$

**Similar formula to 2-body system**

(w/ diagonalization matrix U which includes dynamics)

(non-rela approx.)

# Extension to multi-particle systems ( $n \geq 3$ )

- NBS wave function

S.Aoki et al. (HAL Coll.), PRD88(2013)014036

$$\psi_\alpha([\mathbf{x}]) = {}_{\text{in}} \langle 0 | \phi([\mathbf{x}]) | \alpha \rangle_{\text{in}} = {}_{\text{in}} \langle 0 | N(\vec{x}_1) N(\vec{x}_2) \cdots N(\vec{x}_n) | \alpha \rangle_{\text{in}}$$

Lippmann-Schwinger eq.

$$\psi_\alpha([\mathbf{x}]) = {}_{\text{in}} \langle 0 | \phi([\mathbf{x}]) | \alpha \rangle_0 + \int d\beta \frac{{}_{\text{in}} \langle 0 | \phi([\mathbf{x}]) | \beta \rangle_0 T_{\beta\alpha}}{E_\alpha - E_\beta + i\epsilon}$$

Expansion w/ hyper-coordinate

$$\psi(\mathbf{R}, \mathbf{Q}_A) = \sum_{[L],[K]} \psi_{[L][K]}(\mathbf{R}, \mathbf{Q}_A) Y_{[L]}(\Omega_{\mathbf{R}}) \overline{Y_{[K]}(\Omega_{\mathbf{Q}_A})}$$

$$\psi_{[L],[K]}(\mathbf{R}, \mathbf{Q}_A) \propto \sum_{[N]} U_{[L][N]}(\mathbf{Q}_A) e^{i\delta_{[N]}(\mathbf{Q}_A)} \frac{\sin(\mathbf{Q}_A \mathbf{R} - \Delta_L + \delta_{[N]}(\mathbf{Q}_A))}{(\mathbf{Q}_A \mathbf{R})^{(D-1)/2}} U_{[N][K]}^\dagger(\mathbf{Q}_A)$$

**Similar asymptotic behavior to 2-body system**

(non-rela approx.)

**Extension when subsystem is bound also established !**

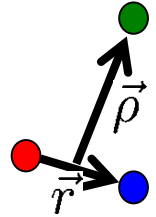
S. Gongyo, S. Aoki,  
PTEP2018(2018)093B03

c.f. Finite V spectrum,  $n=3$  only, relativistic: Hansen, Sharpe, Briceno, Rusetsky, Mai, ...

# Genuine 3NF from HAL QCD method

- Nambu-Bethe-Salpeter (NBS) wave function

$$\psi(\vec{r}, \vec{\rho}) = \langle 0 | N(\vec{x} + \vec{r}) N(\vec{x}) N(\vec{x} + \vec{r}/2 + \vec{\rho}) | 3N \rangle$$



- Obtain 3NF through

$$(E - H_0^r - H_0^\rho) \psi(\vec{r}, \vec{\rho}) = \left[ \underbrace{\sum_{i < j} V_{ij}(\vec{r}_{ij})}_{\substack{\uparrow \\ \text{by 2N calc}}} + V_{3NF}(\vec{r}, \vec{\rho}) \right] \psi(\vec{r}, \vec{\rho})$$

- NBS is obtained by 6pt. correlator

$$G(\vec{r}, \vec{\rho}, t - t_0) = \sum_{\vec{x}} \langle 0 | N(\vec{x} + \vec{r}, t) N(\vec{x}, t) N(\vec{x} + \vec{r}/2 + \vec{\rho}, t) \overline{N N N}(t_0) | 0 \rangle$$

In practical calculation,  
we employ time-dependent HAL QCD method

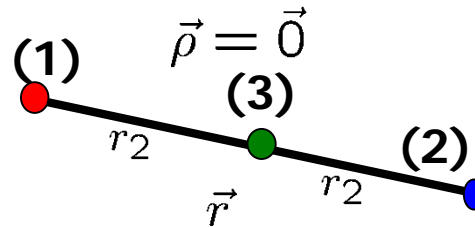
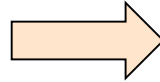
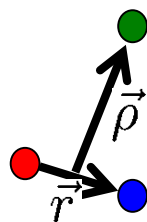
$$\left( -H_0 - \frac{\partial}{\partial t} \right) R(\mathbf{r}, t) = V(r) R(\mathbf{r}, t)$$

N.Ishii et al. (HAL QCD Coll.) PLB712(2012)437

→ Ground state saturation is NOT necessary !

# 3NF calculation in Lat QCD

- We fix the geometry of 3N (← this is not an approximation)
- We study **linear setup**



We consider  
Triton channel

$$(\vec{r}_2 \equiv \vec{r}/2)$$

- →  $L^{(1,2)\text{-pair}} = L^{\text{total}} = 0$  or  $2$  only
- → **Bases are only three**, labeled by  $^1S_0, ^3S_1, ^3D_1$  for (1,2)-pair

$$|\psi_S\rangle = 1/\sqrt{2} (-|\psi_{1S_0}\rangle + |\psi_{3S_1}\rangle)$$

→ L=even for any 2N pair automatically guaranteed

2NF contribution can be obtained only from 2NF(P=even)



# (1) Identification of Genuine 3NF

■ **Genuine 3NF** can be extracted from **3x3 coupled channel**

- Both of parity-even 2NF and parity-odd potential required

$$\hat{H}_0 \begin{pmatrix} \psi(1S_0) \\ \psi(3S_1) \\ \psi(3D_1) \end{pmatrix} + \begin{pmatrix} V \\ (V_{2N} + V_{3NF}) \end{pmatrix} \begin{pmatrix} \psi(1S_0) \\ \psi(3S_1) \\ \psi(3D_1) \end{pmatrix} = E \begin{pmatrix} \psi(1S_0) \\ \psi(3S_1) \\ \psi(3D_1) \end{pmatrix}$$

$V_C^{I,S=1,0}, V_C^{I,S=0,1}, V_T^{I,S=0,1} : (P = \text{even})$

$V_C^{I,S=0,0}, V_C^{I,S=1,1}, V_T^{I,S=1,1} : (P = \text{odd})$

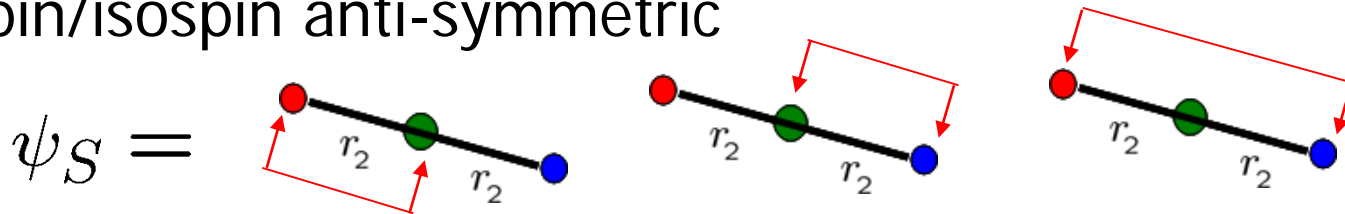
**Target to be determined**

■ S/N : parity-even 2NF > parity-odd 2NF in Lat QCD

- → **Desirable to extract 3NF w/ parity-even 2NF only**

# Solution using “symmetric” wave function

- We can construct the wave function in which any 2N pair is spin/isospin anti-symmetric



- L=even for any 2N pair automatically guaranteed

- Bases are rotated as  $|\psi_{1S_0}\rangle, |\psi_{3S_1}\rangle, |\psi_{3D_1}\rangle \rightarrow |\psi_S\rangle, |\psi_M\rangle, |\psi_{3D_1}\rangle$

$$|\psi_S\rangle = 1/\sqrt{2}(-|\psi_{1S_0}\rangle + |\psi_{3S_1}\rangle)$$

$$|\psi_M\rangle = 1/\sqrt{2}(+|\psi_{1S_0}\rangle + |\psi_{3S_1}\rangle)$$

All pair P=even

$$\hat{H}_0 \begin{pmatrix} \psi_S \\ \psi_M \\ \psi_{3D_1} \end{pmatrix} + \begin{pmatrix} \boxed{\phantom{0}} & \boxed{\phantom{0}} & \boxed{\phantom{0}} \\ \boxed{\phantom{0}} & V_{2N} & \boxed{\phantom{0}} \\ \boxed{\phantom{0}} & \boxed{\phantom{0}} & \boxed{\phantom{0}} \end{pmatrix} \begin{pmatrix} \psi_S \\ \psi_M \\ \psi_{3D_1} \end{pmatrix} + \hat{V}_{3NF} \begin{pmatrix} \psi_S \\ \psi_M \\ \psi_{3D_1} \end{pmatrix} = E \begin{pmatrix} \psi_S \\ \psi_M \\ \psi_{3D_1} \end{pmatrix}$$

No V(P=odd)

# Solution using “symmetric” wave function

- We can construct the wave function in which any 2N pair is spin/isospin anti-symmetric
  - → L=even for any 2N pair automatically guaranteed
- 3x3 coupled channel is reduced to
  - one channel with only 3NF unknown
  - two channels with  $V_C^{I,S=0,0}$ ,  $V_C^{I,S=1,1}$ ,  $V_T^{I,S=1,1}$ , (3NF) unknown

$$\begin{pmatrix} H_0 \\ \psi_S \\ \psi_M \\ \psi_{3D_1} \end{pmatrix} + \begin{pmatrix} V_{2N} \\ \psi_S \\ \psi_M \\ \psi_{3D_1} \end{pmatrix} + \begin{pmatrix} V_{3NF} \\ \psi_S \\ \psi_M \\ \psi_{3D_1} \end{pmatrix} = E \begin{pmatrix} \psi_S \\ \psi_M \\ \psi_{3D_1} \end{pmatrix}$$

No V(P=odd)
Target to be determined

- → Even without parity-odd V, we can determine one 3NF
  - This method works for any fixed 3D-geometry other than linear

# Computational Challenge

- **Enormous comput. cost for multi-baryon correlators**

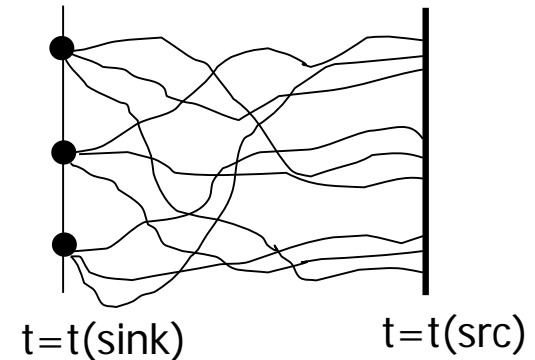
- Wick contraction (permutations)

$$\sim \left[ \left( \frac{3}{2} A \right)! \right]^2 \quad (A: \text{mass number})$$

- color/spinor contractions

$$\sim 6^A \cdot 4^A \quad \text{or} \quad 6^A \cdot 2^A$$

See also T. Yamazaki et al.,  
PRD81(2010)111504



- **Unified Contraction Algorithm (UCA)**

- A novel method which unifies two contractions

$$\Pi^{2N} \simeq \langle qqqqqq(t) \bar{q}(\xi'_1) \bar{q}(\xi'_2) \bar{q}(\xi'_3) \bar{q}(\xi'_4) \bar{q}(\xi'_5) \bar{q}(\xi'_6)(t_0) \rangle \times \text{Coeff}^{2N}(\xi'_1, \dots, \xi'_6)$$

Permuted Sum Sum over color/spinor unified list

## Drastic Speedup

×192 for  ${}^3\text{H}/{}^3\text{He}$ , ×20736 for  ${}^4\text{He}$ , ×10<sup>11</sup> for  ${}^8\text{Be}$

(x add'l. speedup)



# Lattice simulation setup

---

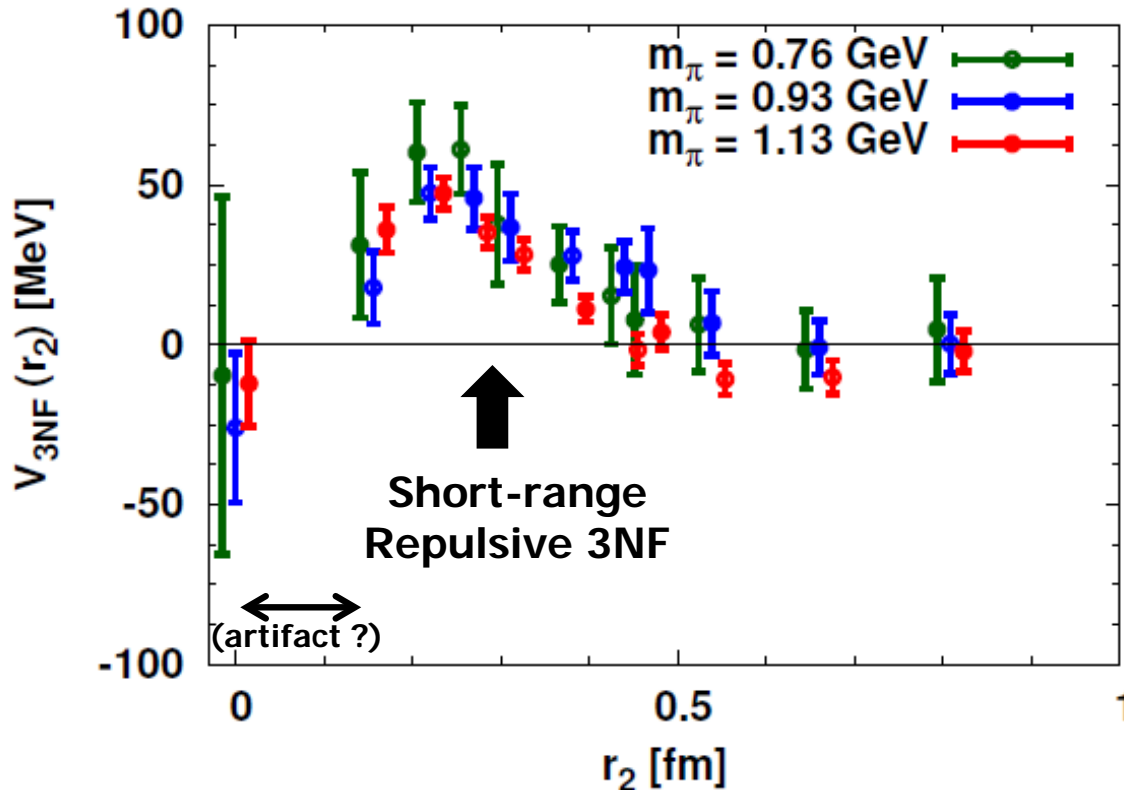
- Nf=2 dynamical clover fermion + RG improved gauge action
  - $a^{-1}=1.269\text{GeV}$ ,  $a=0.1555\text{fm}$  ( $\beta=1.95$ )
  - $16^3 \times 32$  lattice,  $L=2.5\text{fm}$
- Masses:  $(\pi, N, \Delta) = (1.13, 2.15, 2.31) \text{ GeV}$ 
  - $\text{Kappa}(ud)=0.13750$
  - 599 configs x 32 measurements,  $t+1=[5,12]$
- Masses:  $(\pi, N, \Delta) = (0.925, 1.85, 2.02) \text{ GeV}$ 
  - $\text{Kappa}(ud)=0.13900$
  - 686 configs x 32 measurements,  $t+1=[5,12]$
- Masses:  $(\pi, N, \Delta) = (0.757, 1.61, 1.81) \text{ GeV}$ 
  - $\text{Kappa}(ud)=0.14000$
  - 686 configs x 32 measurements,  $t+1=[5,12]$

CP-PACS Coll. S. Aoki et al.,  
Phys. Rev. D65 (2002) 054505

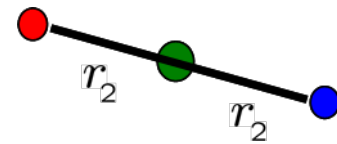
# 3N-forces (3NF) in $m_\pi \geq 0.76$ GeV

T.D. et al. (HAL QCD Coll.) PTP127(2012)723 + t-dep method updates etc.

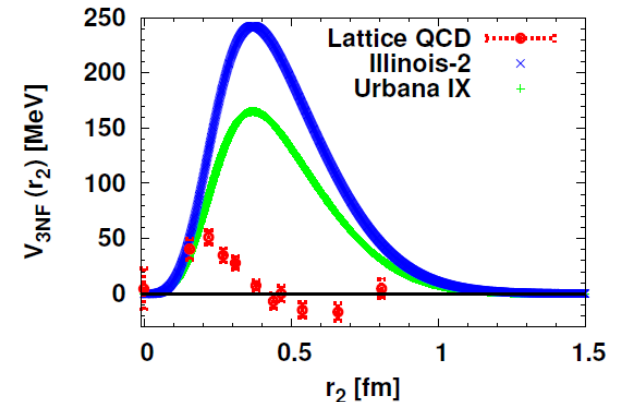
Nf=2 clover (CP-PACS),  $1/a=1.27$  GeV,  
 $L=2.5$  fm,  $m_\pi=0.76-1.1$  GeV,  $m_N=1.6-2.1$  GeV



Triton channel



Naïve comparison to phenomenological 3NF

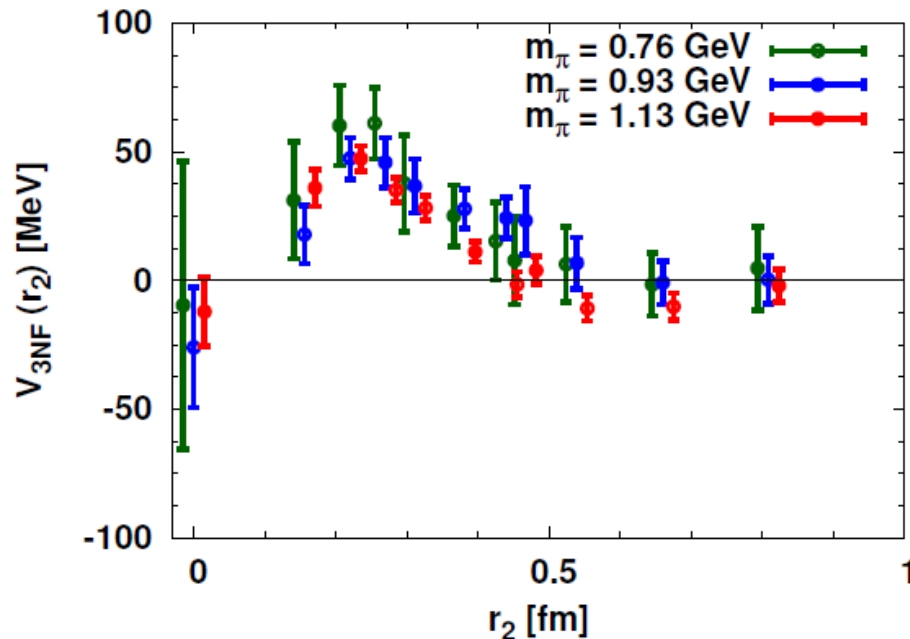


(t-t0 = 7.5)

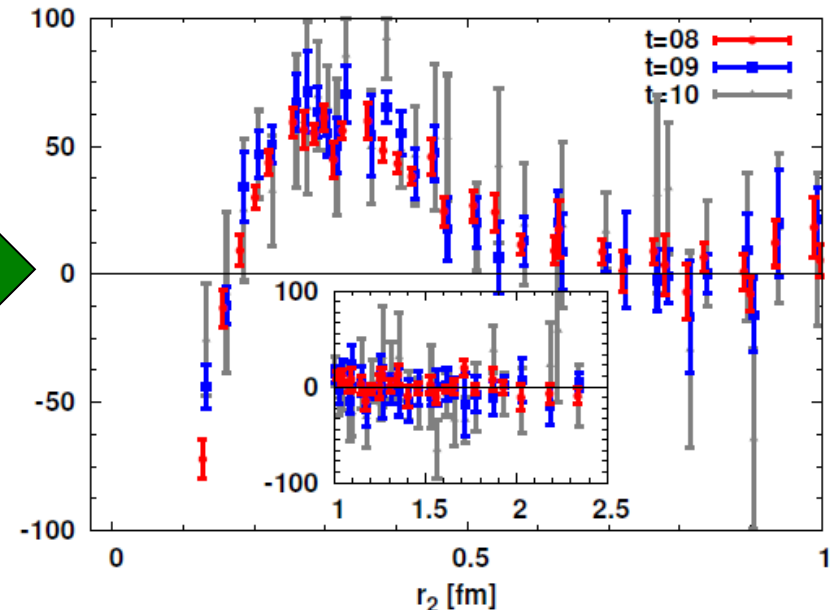
→ Lighter quark mass important ?

# Towards lighter quark masses

$N_f=2, m_\pi=0.76-1.1$  GeV



$N_f=2+1, m_\pi=0.51$  GeV



Magnitude of 3NF is similar for all masses  
Range of 3NF tend to be enlarged for  $m(\pi)=0.5$ GeV

Next challenge: **Calc of P-wave 2BF** : better subtraction of 2BF in 3-body systems  
**YNN** (w/o or w/ P-wave 2BF) : gauge conf generation on Fugaku

# P-wave 2NF int by all-to-all method

## LapH method

M. Peardon et al., PRD80(2009)054506

$$S^{ab}(x, y) = \sum_{l=0}^{N_l} \omega_l v_l^a(x) v_l^{*b}(y)$$

$$\Delta^{ab}(x, y; U) = \sum_{k=1}^3 \left\{ U_k^{ab}(x) \delta(y, x + \hat{k}) + U_k^{ba}(y)^* \delta(y, x - \hat{k}) - 2\delta(x, y) \delta^{ab} \right\}$$
$$= \begin{pmatrix} \mathbf{v}_1 & \mathbf{v}_2 & \cdots & \mathbf{v}_N \end{pmatrix} \begin{pmatrix} \lambda_1 & & & \mathbf{0} \\ & \lambda_2 & & \\ & & \ddots & \\ \mathbf{0} & & & \lambda_N \end{pmatrix} \begin{pmatrix} \mathbf{v}_1^\dagger \\ \mathbf{v}_2^\dagger \\ \vdots \\ \mathbf{v}_N^\dagger \end{pmatrix}$$

Approximate all-to-all prop by  $N_l$  low-modes in gauge covariant Laplacian

## New improvement: Free LapH method

gauge cov. Laplacian  $\rightarrow$  free Laplacian

$$\Delta(x, y) = \sum_{k=1}^3 \left\{ \delta(y, x + \hat{k}) + \delta(y, x - \hat{k}) - 2\delta(x, y) \right\}$$

Comput. Cost can be reduced from  $O(N_c^4 \times N_l^4) \rightarrow N_c! N_c O(N_l^3)$

[\$\rightarrow\$  Typically  \$O\(100\)\$  speedup!](#)

Explicit calc for NN in progress

[T. Sugiura]

$\rightarrow$  P-wave int, LS-forces, better systematics



# Summary

- Hadron Int.: Bridge between particle/nuclear/astro-physics
- HAL QCD method for LQCD determination of Hadron Int.
  - The “potential” can be defined in QFT even for three- (and multi-) body forces
- **Three-Nucleon Forces**
  - Method to extract 3NF in  $I=1/2$  channel
  - Short-range repulsion observed for  $m(\pi) = 0.51\text{GeV}, 0.76\text{-}1.13\text{GeV}$
- Prospects
  - P-wave 2NF in progress  $\rightarrow$  3NF in  $I=3/2$  channel
  - 3BF w/ hyperons  $\rightarrow$  EoS of dense matter



Fugaku (440PFlops)

