

# QCD in finite volume

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# Lecture 3

# Outline, lecture 3

- interpolators
- Wick contractions
- all-to-all propagators: distillation method
- Applications:
  - bound states
  - virtual bound states
  - resonances (covered in lecture 4)

In all cases : energy regions where a single channel  $H_1 H_2$  is present

# Interpolators

they create/annihilate states of the system with given quantum number (irrep /  $J^{PC}$ )

meson example (of course quarks  $q$  can have different flavors)

$$\bar{q}(0) \Gamma D_i D_j q(0)$$

$$\sum_{\vec{x}} \bar{q}(\vec{x}) \Gamma D_i D_j q(\vec{x}) e^{i\vec{P}\vec{x}}$$

$$\sum_j M_1(\vec{p}_{1j}) \quad M_2(\vec{p}_{2j})$$

$$\sum_j \sum_{\vec{x}} \bar{q}(\vec{x}) \Gamma_{1j} q(\vec{x}) e^{i\vec{p}_{1j}\vec{x}} \quad \sum_{\vec{y}} \bar{q}(\vec{y}) \Gamma_{2j} q(\vec{y}) e^{i\vec{p}_{2j}\vec{y}}$$

$$\sum_{\vec{x}} [\bar{q}(\vec{x}) \Gamma_1 \bar{q}(\vec{x})]_{3_c} [q(\vec{x}) \Gamma_2 q(\vec{x})]_{\bar{3}_c} e^{i\vec{P}\vec{x}}$$

# Wick contractions: all-to-all propagators needed

example of M1 M2 ↔ M1 M2 contraction

$O(t_f)$

$O(t_i)$

$$\sum_j M_1(\vec{p}_{1j}, t_f) \quad M_2(\vec{p}_{2j}, t_f) \quad \sum_j M_1(\vec{p}_{1j}, t_i) \quad M_2(\vec{p}_{2j}, t_i)$$

$$\sum_j \sum_{\vec{x}_f} \bar{q}(\vec{x}_f, t_f) \Gamma_{1j} q(\vec{x}_f, t_f) e^{i\vec{p}_{1j} \vec{x}_f} \quad \sum_{\vec{y}_f} \bar{q}(\vec{y}_f, t_f) \Gamma_{2j} q(\vec{y}_f, t_f) e^{i\vec{p}_{2j} \vec{y}_f} \quad \sum_j \sum_{\vec{x}_i} \bar{q}(\vec{x}_i, t_i) \Gamma_{1j} q(\vec{x}_i, t_i) e^{i\vec{p}_{1j} \vec{x}_i} \quad \sum_{\vec{y}_i} \bar{q}(\vec{y}_i, t_i) \Gamma_{2j} q(\vec{y}_i, t_i) e^{i\vec{p}_{2j} \vec{y}_i}$$

$$q(\vec{x}_f, t_f) \bar{q}(\vec{x}_i, t_i)$$

Propagators from all points  $x_i, t_i$  to all points  $x_f, t_f$  needed

$$\sum_j M_1(\vec{p}_{1j}, t_f) \quad M_2(\vec{p}_{2j}, t_f)$$

$$\sum_j \sum_{\vec{x}_f} \bar{q}(\vec{x}_f, t_f) \Gamma_{1j} q(\vec{x}_f, t_f) e^{i\vec{p}_{1j} \vec{x}_f} \quad \sum_{\vec{y}_f} \bar{q}(\vec{y}_f, t_f) \Gamma_{2j} q(\vec{y}_f, t_f) e^{i\vec{p}_{2j} \vec{y}_f}$$

if those two are of same flavor

$$q(\vec{x}_f, t_f) \bar{q}(\vec{y}_f, t_f)$$

$$\sum_j M_1(\vec{p}_{1j}, t_i) \quad M_2(\vec{p}_{2j}, t_i)$$

$$\sum_j \sum_{\vec{x}_i} \bar{q}(\vec{x}_i, t_i) \Gamma_{1j} q(\vec{x}_i, t_i) e^{i\vec{p}_{1j} \vec{x}_i} \quad \sum_{\vec{y}_i} \bar{q}(\vec{y}_i, t_i) \Gamma_{2j} q(\vec{y}_i, t_i) e^{i\vec{p}_{2j} \vec{y}_i}$$

Propagators from all points  $y_f, t_f$  to all points  $x_f, t_f$  needed

Brute force: this would require calculation propagators from all  $(x,t)$  space time points:  $N_L^3 \times N_T \times 3$  inversions.

In practice: this is not feasible

(for each Dirac index)

- **Distillation method for all-to-all propagators**

most-weidely employed method to get all-to-all propagators:

distillation method: [Peardon et al 2009 \*Phys.Rev.D\* 80 \(2009\) 054506](#)

I suggest to read the original reference to learn the method

$$q(\vec{x}, t) \rightarrow q_s(\vec{x}, t)$$

spatially-smearred quark around point x

$$q_s^{\alpha c}(\vec{x}, t) = \sum_{k=1}^{k=N_v} v_{\vec{x}c}^{(k)}(t) v_{\vec{x}'c'}^{(k)\dagger}(t) q^{\alpha c'}(\vec{x}', t)$$

spectral decomposition



Laplace Heaviside smearing (cuts-out higher frequency modes)

$v^{(k)}(t)$   $k=1, \dots, N$  are eigenvectors of lattice Laplace-operator(t) which is  $N \times N$  matrix,  $N=3 N_L^3$

if  $N_v=N$  :  $q_s=q$ ,  $N_v=O(100) \ll 3 N_L^3$  is taken

# Distillation method for all-to-all propagators

number of inversions per Dirac index

brute force: propagators from all  $x_i, t_i$  to all  $x_f, t_f$

$$3 \times N_L^3 \times N_T$$

$$q(\vec{x}_f, t_f) \bar{q}(\vec{x}_i, t_i)$$

(not feasible)

distillation : propagators from  $v^{(k_i)}(t_i)$  ( $k_i=1,\dots,N_v$ ) to  $v^{(k_f)}(t_f)$  ( $k_f=1,\dots,N_v$ )

$$3 \times N_v, \quad N_v \sim O(100)$$

$$\tau^{k_f k_i}(t_f, t_i) \equiv v^{(k_f)}(t_f) v^{(k_i)\dagger}(t_i)$$

these propagators are calculated and stored

they are called peramulators

all Wick contractions can be expressed in terms of them

(as long as one is happy with using smeared quarks)

for matrix elements of local currents one needs point-quarks  $\langle H_f | \bar{q}(x) \Gamma q(x) | H_i \rangle$

# Reminder how to identify on the lattice bound state, virtual bound state, resonances

$$T = \frac{1}{p \cot \delta_l - ip}$$

Scattering of two hadrons H1 H2

- assuming that only one channel is present in the given energy region (elastic scattering)
- H1 H2 carry no spin

- Determine eigen-energies  $E$ ,  $E=E_{\text{cm}}$
- Determine  $T_l(E)$  for these  $E$  via Luscher's equation

Riemann sheet I if  $\text{Im}(p)>0$ , Riemann sheet II if  $\text{Im}(p)<0$        $E = \sqrt{m_1^2 + p^2} + \sqrt{m_2^2 + p^2}$

- location of pole in the scattering amplitude  $T(E)$  help to identify

bound state: pole for real  $E$  below threshold      Riemann sheet I

virtual bound state: pole for real  $E$  below threshold Riemann sheet II

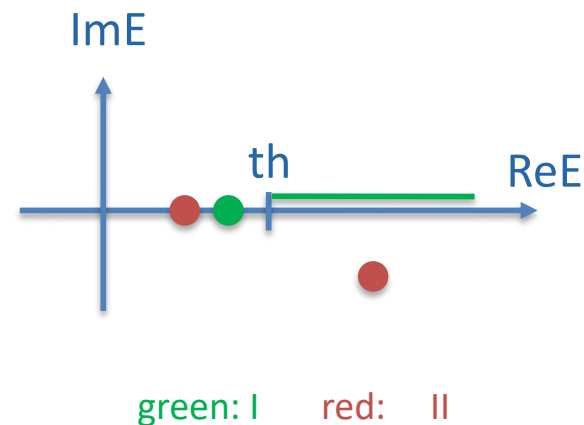
no need to consider complex  $E$  for (virtual) bound states

- for resonances :  $T(\text{real } E) \rightarrow T(\text{complex } E)$

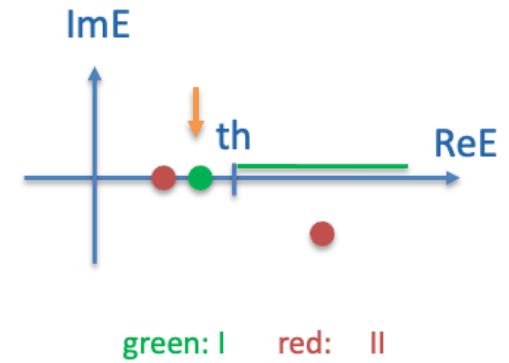
resonance: pole away from real axes  $E = m - 1/2 i \Gamma$       Riemann sheet II

these poles affect physical scattering ("peaks in  $\sigma$ ")

if they are close to physical axes (green line)      Riemann sheet I







## Shallow bound states

pole of  $T(E)$  for real  $E$  below threshold

$p=i|p|$  : Riemann sheet I

# $D_{s0}^*$ shallow bound state in DK scattering: $l=0, J^P=0^+$

$D_{s0}^*$  lies 45 MeV below DK strong decay threshold in experiment

Mode		Fraction ( $\bar{\Gamma}_i / \Gamma$ )
$\Gamma_1$	$D_s^+ \gamma$	$(93.5 \pm 0.7)\%$
$\Gamma_2$	$D_s^+ \pi^0$	$(5.8 \pm 0.7)\%$
$\Gamma_3$	$D_s^+ e^+ e^-$	$(6.7 \pm 1.6) \times 10^{-3}$

D. Mohler, C. Lang, L. Leskovec, S.P., R. Woloshyn: Phys. Rev. Lett. 2013, PRD 2014

$m_\pi=156$  MeV,  $N_f=2+1$ ,  $V=32^3 \times 64$ ,  $L=2.9$  fm [PACS-CS] PACSCS

$P_{\text{tot}}=0$  : interpolators in irrep  $A_1^+$  of Oh contain  $J=0$  states

$$O^{qq} = \bar{s}c \quad (p=0)$$

$$\bar{s}\gamma_i\nabla_i c$$

$$\bar{s}\gamma_t\gamma_i\nabla_i c$$

$$\bar{s}\nabla_i\nabla_i c$$

$$O_1^{DK} = [\bar{s}\gamma_5 u] (\vec{p}=0) [\bar{u}\gamma_5 c] (\vec{p}=0) + \{u \rightarrow d\} ,$$

$$O_2^{DK} = [\bar{s}\gamma_t\gamma_5 u] (\vec{p}=0) [\bar{u}\gamma_t\gamma_5 c] (\vec{p}=0) + \{u \rightarrow d\}$$

$$O_3^{DK} = \sum_{\vec{p}=\pm e_{x,y,z} 2\pi/L} [\bar{s}\gamma_5 u] (\vec{p}) [\bar{u}\gamma_5 c] (-\vec{p}) + \{u \rightarrow d\} .$$

C evaluated using distillation method [Peardon et al.]

$$C_{ij}(t) = \langle 0 | O_i(t) O_j^\dagger | 0 \rangle = \sum_k Z_{ik}^\dagger Z_{kj} e^{-E_k t}$$

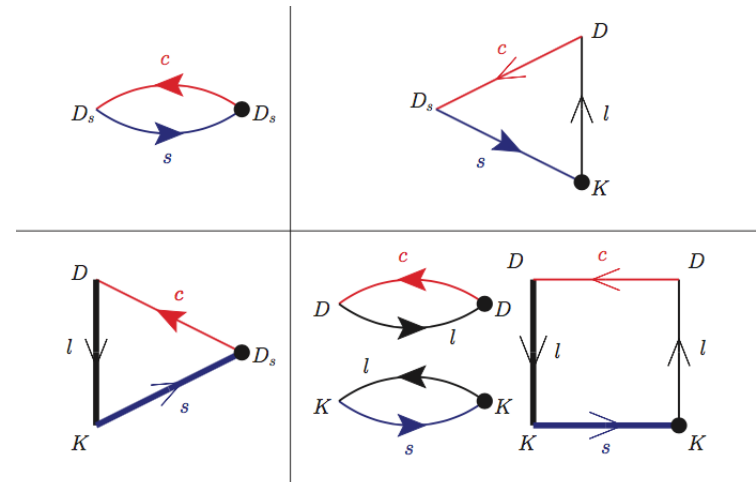
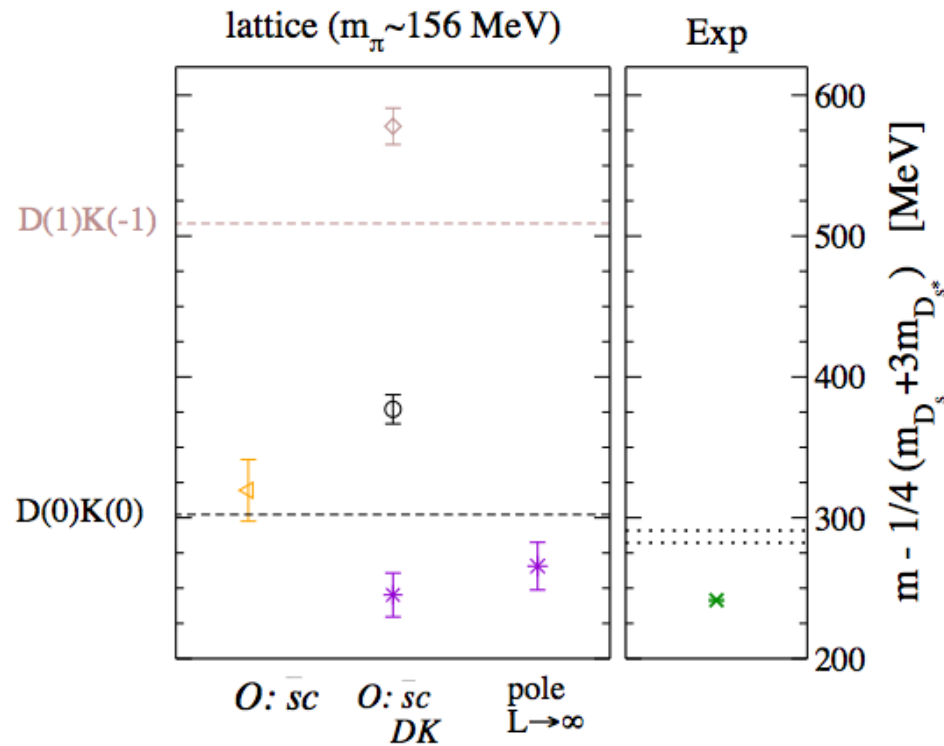


Figure by RQCD

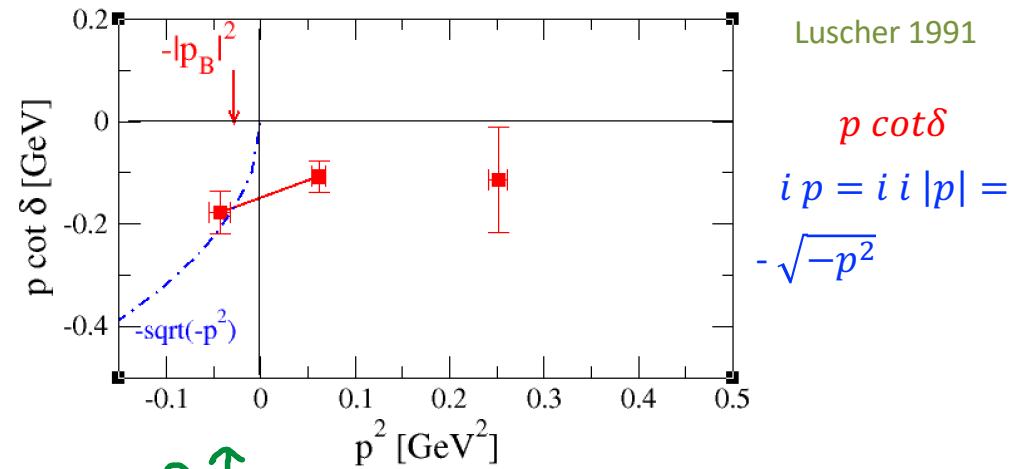
# $D_{s0}^*(2317)$



D. Mohler, C. Lang, L. Leskovec, S.P., R. Woloshyn:  
 Phys. Rev. Lett. 2013:  $m_\pi \approx 156$  MeV,  $L \approx 2.9$  fm,  $N_f=2+1$ , PACSCS  
 mesonic bound st. established on lattice for the first time

$D_{s0}^*(2317)$	$m - 1/4 (m_{D_s} + 3m_{D_s^*})$	$m_D + m_K - m$
lat	$266 \pm 16 \pm 4$ MeV	$36 \pm 17$ MeV
exp	$241.45 \pm 0.6$ MeV	45 MeV

$$E = \sqrt{m_D^2 + p^2} + \sqrt{m_K^2 + p^2} \quad p \cot \delta(p) = \frac{2}{\sqrt{\pi}L} Z_{00}(1, (\frac{pL}{2\pi})^2)$$



$$p \cot \delta(p) = \frac{1}{a_0} + \frac{1}{2} r_0 p^2$$

$$a_0 = -1.33 \pm 0.20 \text{ fm} \quad r_0 = 0.27 \pm 0.17 \text{ fm}$$

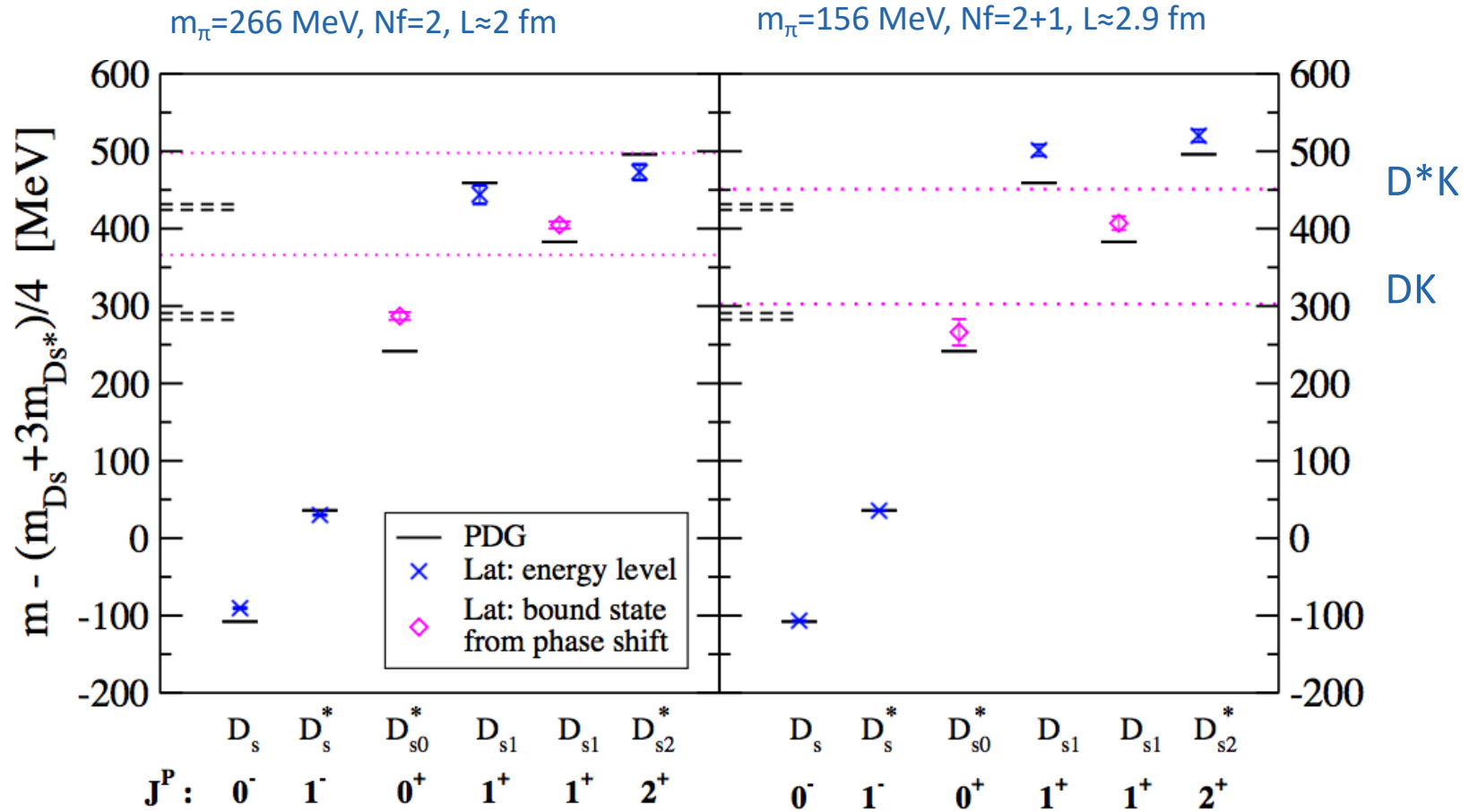
$$T = \frac{1}{p \cot \delta_0 - ip}$$

$$i p_B = p_B \cot \delta(p_B), \quad p_B = i |p_B|$$

$$i |p_B| * i = \frac{1}{a_0} - \frac{1}{2} r_0 |p_B|^2 \rightarrow |p_B|^2 = 0.028 \pm 0.012 \text{ GeV}^2$$

$$m_{D_{s0}}^{lat, L \rightarrow \infty} = \sqrt{m_D^2 - |p_B|^2} + \sqrt{m_K^2 - |p_B|^2}$$

# Spectrum of Ds mesons



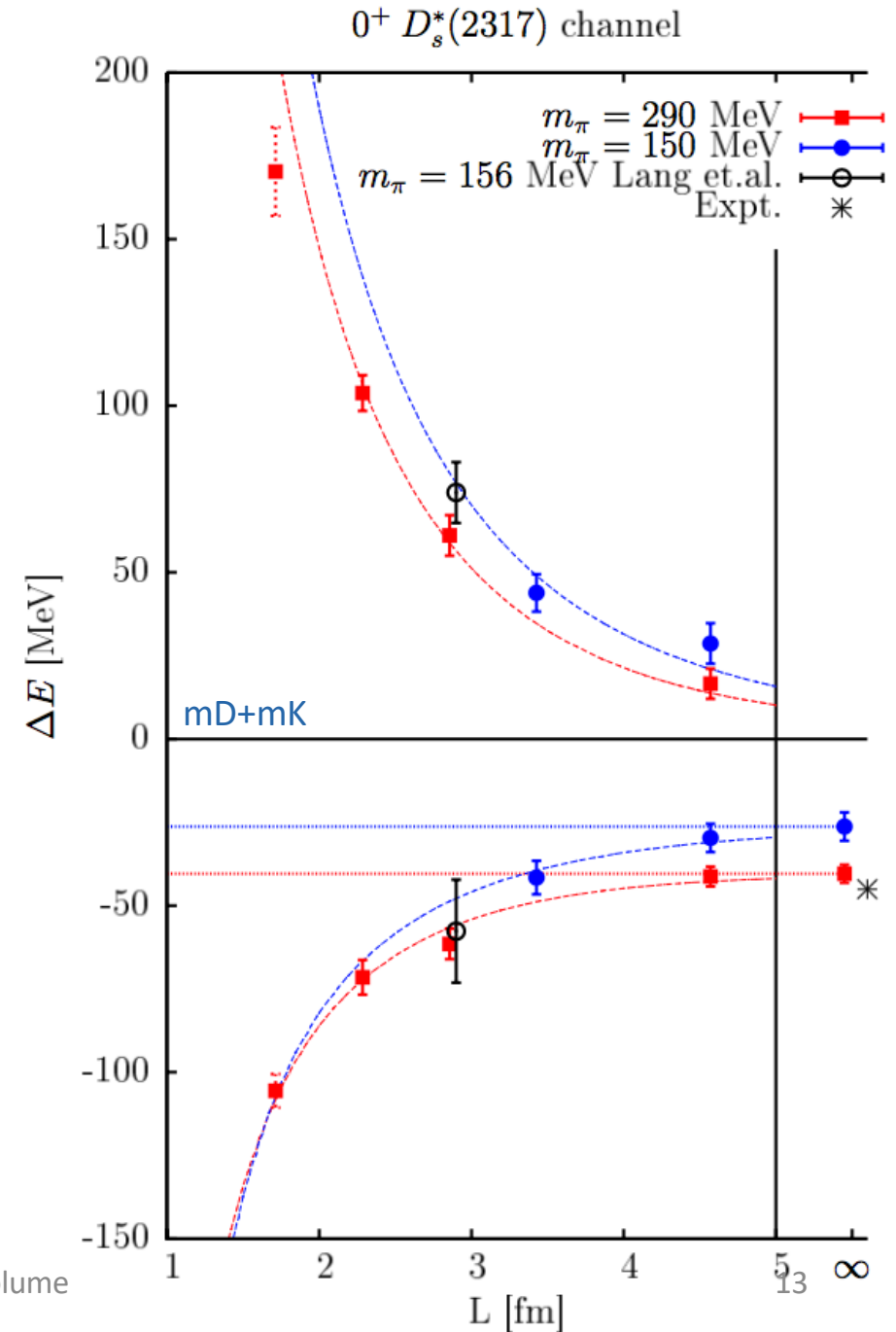
Lang, Leskovec, Mohler, S.P., Woloshyn: PRD 2014, Phys. Rev. Lett. 2013

# $D_{s0}^*(2317)$

Bali, Collins, Cox, Schafer (RQCD):  
PRD (2017) 074501

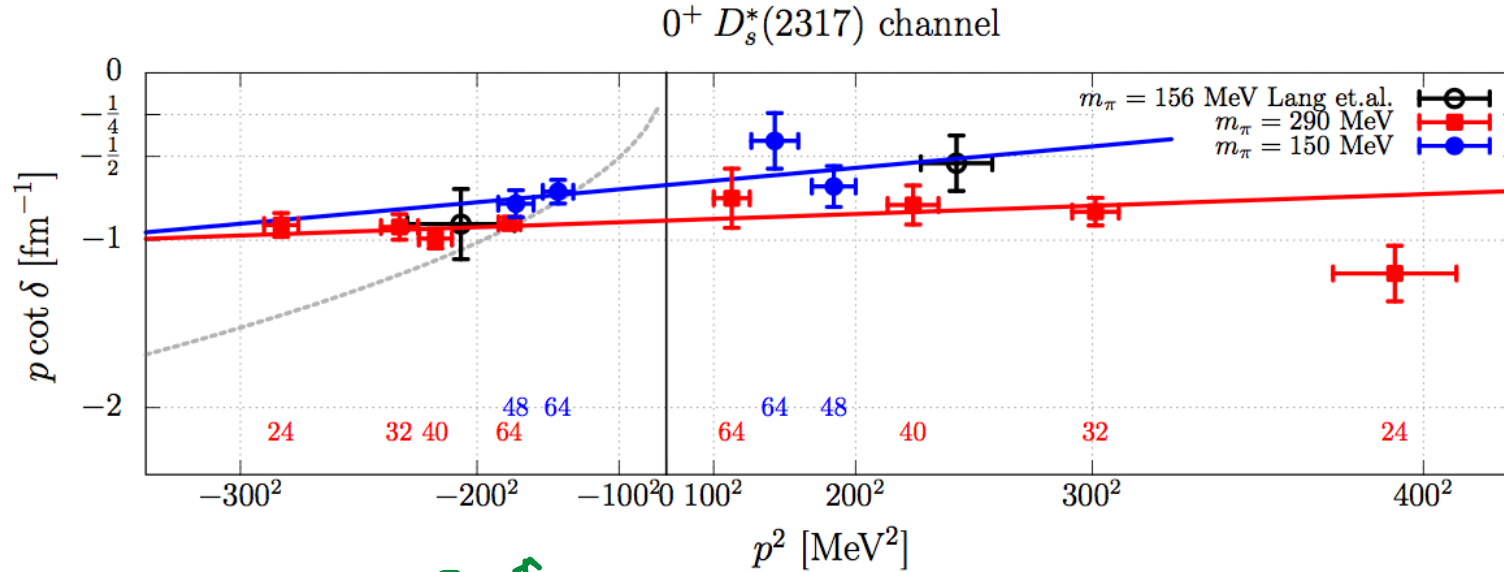
$\kappa_l$	$a$ [fm]	$V$	$am_\pi$	$m_\pi$ [MeV]
0.13632	0.071	$24^3 \times 48$	0.1112(9)	306.9(2.5)
	0.071	$32^3 \times 64$	0.10675(52)	294.6(1.4)
	0.071	$40^3 \times 64$	0.10465(38)	288.8(1.1)
	0.071	$64^3 \times 64$	0.10487(24)	289.5(0.7)
0.13640	0.071	$48^3 \times 64$	0.05786(55)	159.7(1.5)
	0.071	$64^3 \times 64$	0.05425(49)	149.7(1.4)

$O$ :  $\bar{s}c, D(0)K(0), D(1)K(-1)$



# $D_{s0}^*(2317)$

$O: \bar{s}c, D(0)K(0), D(1)K(-1)$



$$p \cot \delta(p) = \frac{1}{a_0} + \frac{1}{2} r_0 p^2$$

$B \uparrow$

$0^+$  channel

	$m_\pi = 290$ MeV	$m_\pi = 150$ MeV	Expt.	$m_\pi = 156$ MeV
$a_0$ [fm]	-1.13(0.04)(+0.05)	-1.49(0.13)(-0.30)		-1.33(20)
$r_0$ [fm]	0.08(0.03)(+0.08)	0.20(0.09)(+0.31)		0.27(17)
$ p_B $ [MeV]	180(6)(0)	142(11)(-9)		
$\Delta m$ [MeV]	40(3)(0)	26(4)(-3)	42.6(0.7)(2.0)	36 (17)
$m_{D_s}$ [MeV]	2384(2)(-1)	2348(4)(+6)	2317.7(0.6)(2.0)	



# The need for systems with nonzero total momentum $\vec{P}$

So far we considered only  $P=0$ : this renders only  $T(E_{cm})$  at few values of  $E_{cm}$

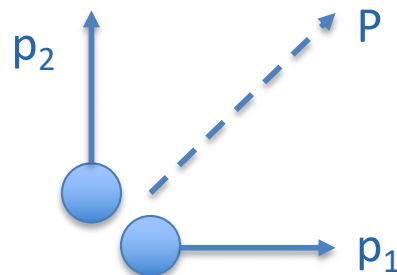
in the non-interacting limit one can reach the following  $E_{cm}$  of  $H_1H_2$

$$P=0 \quad E_{cm} = \sqrt{p^2 + m_1^2} + \sqrt{(-p)^2 + m_2^2}, \quad \vec{p} = \vec{n} \frac{2\pi}{L}$$



$$\text{general } P \quad E = \sqrt{\vec{p}_1^2 + m_1^2} + \sqrt{(\vec{P} - \vec{p}_1)^2 + m_2^2}, \quad \vec{p}_1 = \vec{n} \frac{2\pi}{L}, \quad \vec{P} = \vec{d} \frac{2\pi}{L}$$

$$E_{cm} = \sqrt{E^2 - \vec{P}^2}$$



typical  $P$  considered:

$P=(0,0,1), (1,1,0), (1,1,1) \dots$

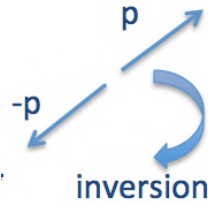
these give access to

additional  $E_{cm}$  and additional  $T(E_{cm})$

# Symmetries are significantly reduced for $P \neq 0$

## continuum

Parity: NOT good



Rotations/reflections:

transformations that leave P invariant  
rotations around P; little group U(1)

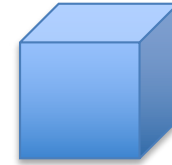
single-particle with momentum P and spin S:  
spin S of a particle: not good  
only  $J=S+L$  : good

helicity : good

$$\lambda = \frac{\vec{S} \cdot \vec{P}}{|\vec{P}|}$$

## cubic lattice

Parity: NOT good



Rotations/reflections:

transformations that leave box and P invariant: Not much symmetry left !!  
(or symmetries of box seen in moving frame)  
 $P=(0,1,0)$ : 8 elements



Irrep	$I$	$R(\pi)$	$R(3\pi/2)$	$R(\pi/2)$	$\Pi$	$R(\pi)\Pi$	$R(\pi/2)\Pi$	$R(3\pi/2)\Pi$
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$P=(1,1,0)$ ; 4 elements

Irrep	$I$	$R(\pi)$	$\Pi$	$R(\pi)\Pi$
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irreps: good quantum numbers  
helicity: not good

challenge: certain irrep gets contribution from both parities and  
several partial waves



# Luscher's relation for $P=0$

$$\det [1 + i\mathcal{M}(E)\mathcal{G}(E)] = 0, \quad E=E_{\text{cm}}$$

$$\mathcal{G}_{l_1, m_1; l_2, m_2}(E) = \frac{p}{8\pi E} \left[ \delta_{l_1, l_2} \delta_{m_1, m_2} + i \sum_{l, m} \frac{(4\pi)^2}{p^{l+1} L^3} \left(\frac{2\pi}{L}\right)^{l-2} Z_{lm} \left(1; \left(\frac{pL}{2\pi}\right)^2\right) \int d\Omega Y_{l_1, m_1}^* Y_{l, m}^* Y_{l_2, m_2} \right]$$

# Generalization of Luscher's relation for $P \neq 0$

$m_1=m_2$ : Rummikainen, Gottlieb 1995 [hep-lat/9503028], Kim, Sachrajda, Sharpe 2005 [hep-lat/0507006]

$m_1 \neq m_2$ : Leskovec & S.P. [1202.2145], Briceno 1401.3312

$$\det[1 + i\mathcal{M}(E_{\text{cm}})\mathcal{G}(E_{\text{cm}})] = 0 \quad p=\text{momentum in cm frame}$$

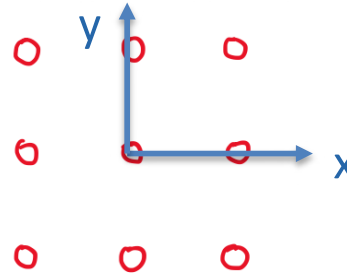
$$\mathcal{G}_{l_1, m_1; l_2, m_2}(E_{\text{cm}}) = \frac{p}{8\pi E_{\text{cm}}} \left[ \delta_{l_1, l_2} \delta_{m_1, m_2} + i \sum_{l, m} \frac{(4\pi)^2}{p^{l+1} L^3} \left(\frac{2\pi}{L}\right)^{l-2} Z_{lm}^{\vec{d}} \left(1; \left(\frac{pL}{2\pi}\right)^2\right) \int d\Omega Y_{l_1, m_1}^* Y_{l, m}^* Y_{l_2, m_2} \right]$$

$$M_l(E) \equiv 8\pi E T_l(E) \quad T_l = \frac{1}{p \cot \delta_l - ip} \quad Z_{lm}^{\vec{d}}(1, q^2) \equiv \sum_{\vec{r} \in P_{\vec{d}}} \frac{r^l Y_{lm}(\vec{r})}{(r^2 - q^2)}$$

$$Z_{lm}^{\vec{d}}(1, q^2) \equiv \sum_{\vec{r} \in P_{\vec{d}}} \frac{r^l Y_{lm}(\vec{r})}{(r^2 - q^2)}$$

$$\vec{r} = \vec{n} \in N^3$$

### Symmetries for P=0: O<sub>h</sub>

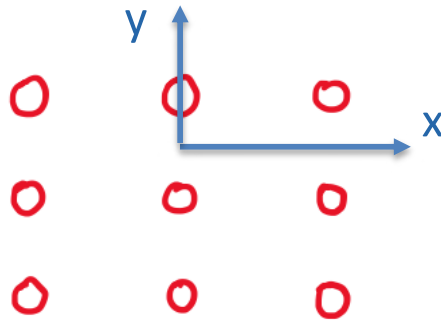


$$\vec{r} \frac{2\pi}{L} = \vec{p} = \hat{\gamma}^{-1}(\vec{p}_1 - \frac{1}{2}A\vec{P})$$

$$\vec{p}_1 = \vec{n} \frac{2\pi}{L}, \quad A = 1 + \frac{m_1^2 - m_2^2}{E_{cm}^2}$$

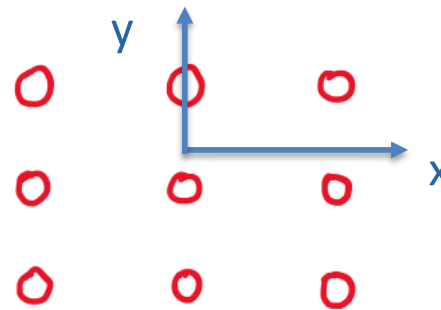
### Symmetries for P ≠ 0

P=(0,1,0) m<sub>1</sub>=m<sub>2</sub>



mesh P<sub>d</sub> invariant under inversion  
 irrep gets contribution of a certain parity  
 irrep gets contribution of only even l  
 or only odd l

P=(0,1,0) m<sub>1</sub> ≠ m<sub>2</sub>



mesh P<sub>d</sub> invariant NOT under inversion  
 irrep gets contribution of both parities (in general, there are fortunately exceptions)  
 irrep gets contribution of even l AND odd l (in general, there are fortunately exceptions)

both meshes are Lorentz contracted in y-direction

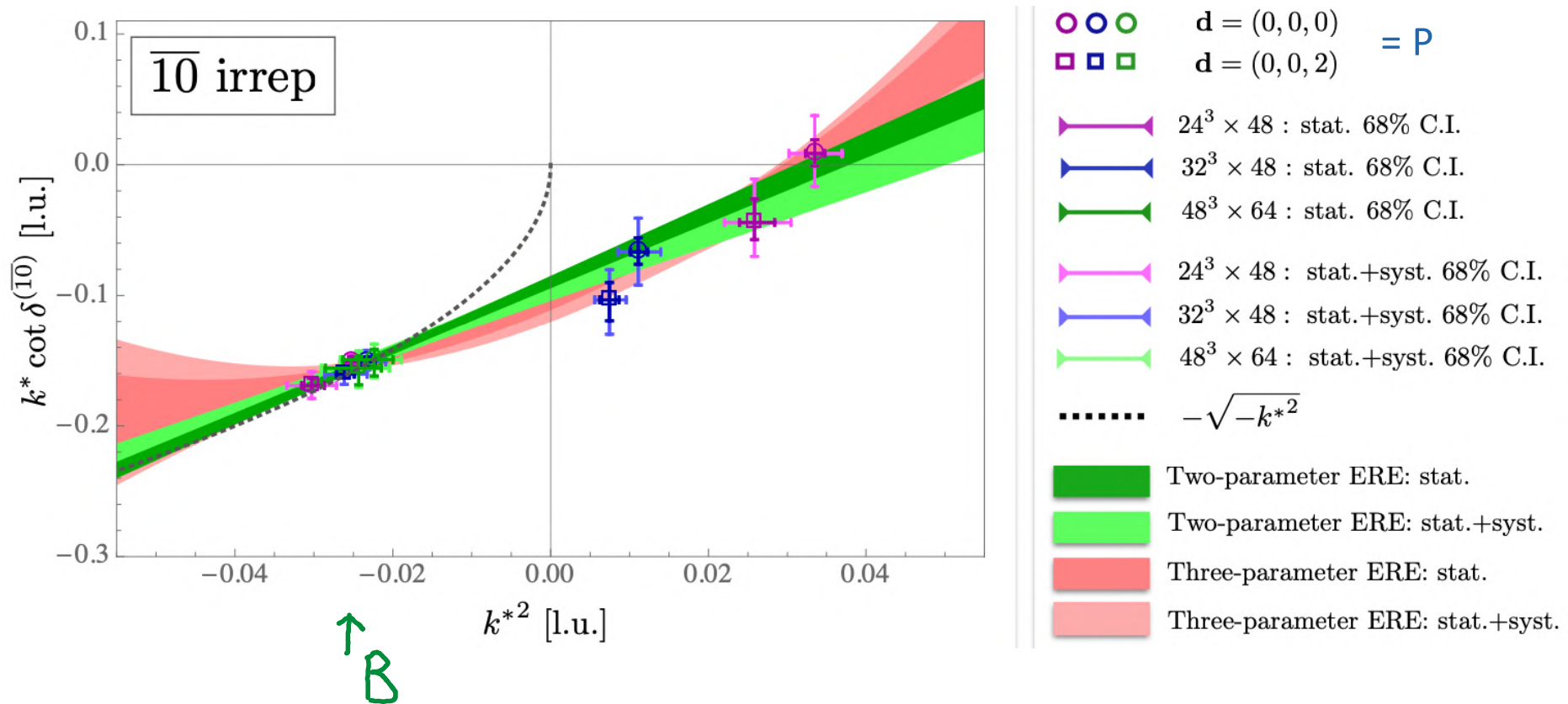
## back to shallow bound states

now with simulations with  $P=0$  and  $P \neq 0$

# Deuteron (pn) channel at $m_u=m_d=m_s$

p,n carry spin: more on scattering in such case in lecture 4

NPLQCD, 1706.0655:  $m_\pi \approx 800\text{MeV}$  :  $m - m_p - m_n = -28(4)\text{MeV}$

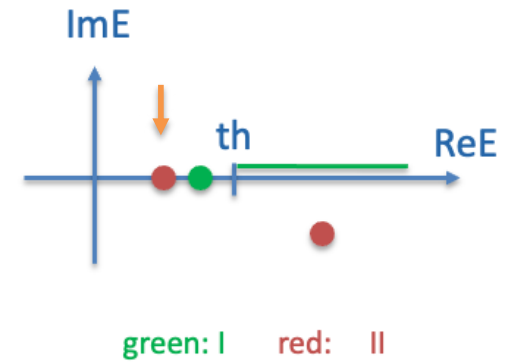


See also results by other groups: HALQCD, Mainz, Callat, Hartz et al,...

lattice groups find inconsistent results (even for SU(3) symmetric case):

some find bound state and some not

exp:  $m - m_p - m_n = -2 \text{ MeV}$



## Virtual bound states

pole of  $T(E)$  for real  $E$  below threshold

$p = -i|p|$  : Riemann sheet II

These are not proper normalizable states

They are features of interaction

# Dineutron (nn) channel at $m_u=m_d=m_s$

n carries spin: more on scattering in such case in lecture 4

Hortz et al, 2009:11825  $m_\pi \approx 714$  MeV

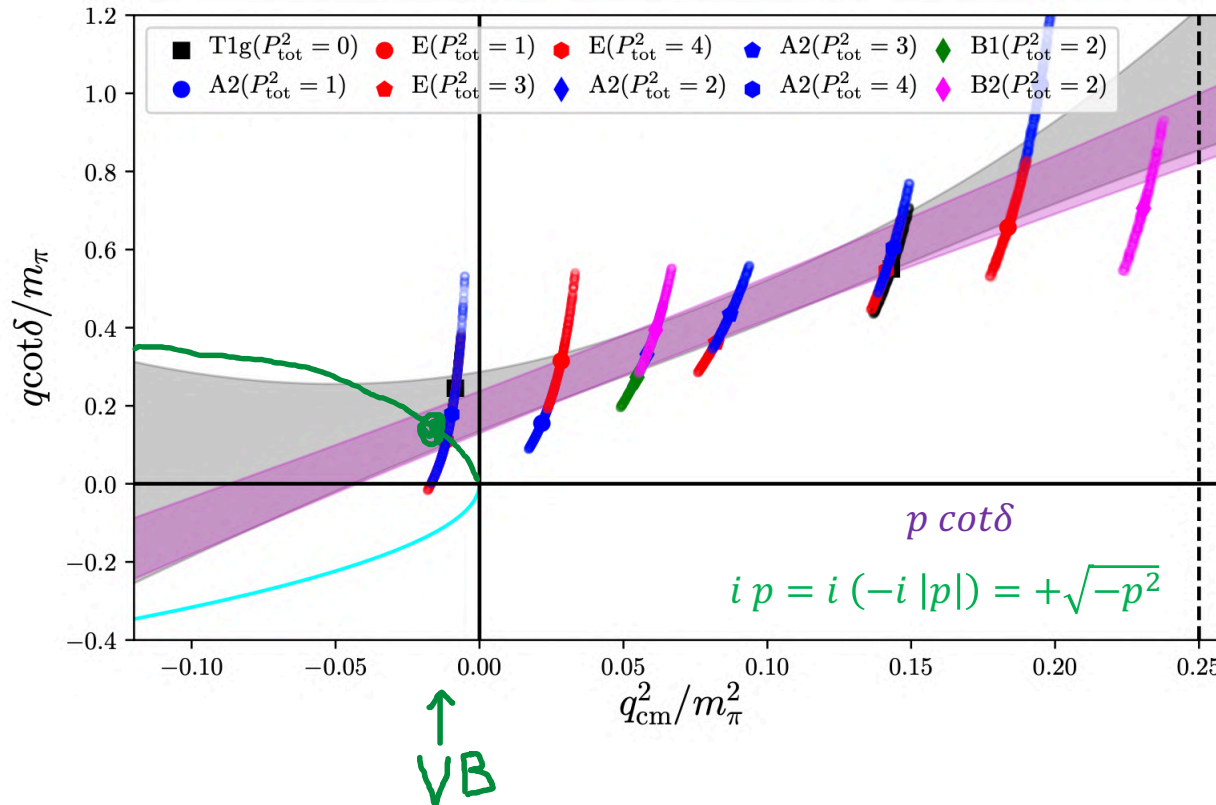
$$T = \frac{1}{p \cot \delta_0 - ip}$$

$$ip = p \cot \delta_0, p = -i|p|$$

$$i(-i|p|) = \frac{1}{a_0} - \frac{1}{2}r_0|p|^2$$

$$m_B = 2\sqrt{m_n^2 - |p|^2} = ?$$

exp:  $m - 2m_n = -60$  keV



See also results by other groups: HALQCD, Mainz, Callat, Hortz et al, ...  
 lattice groups find inconsistent results (even for SU(3) symmetric case):  
 some find virtual bound state and some find bound state

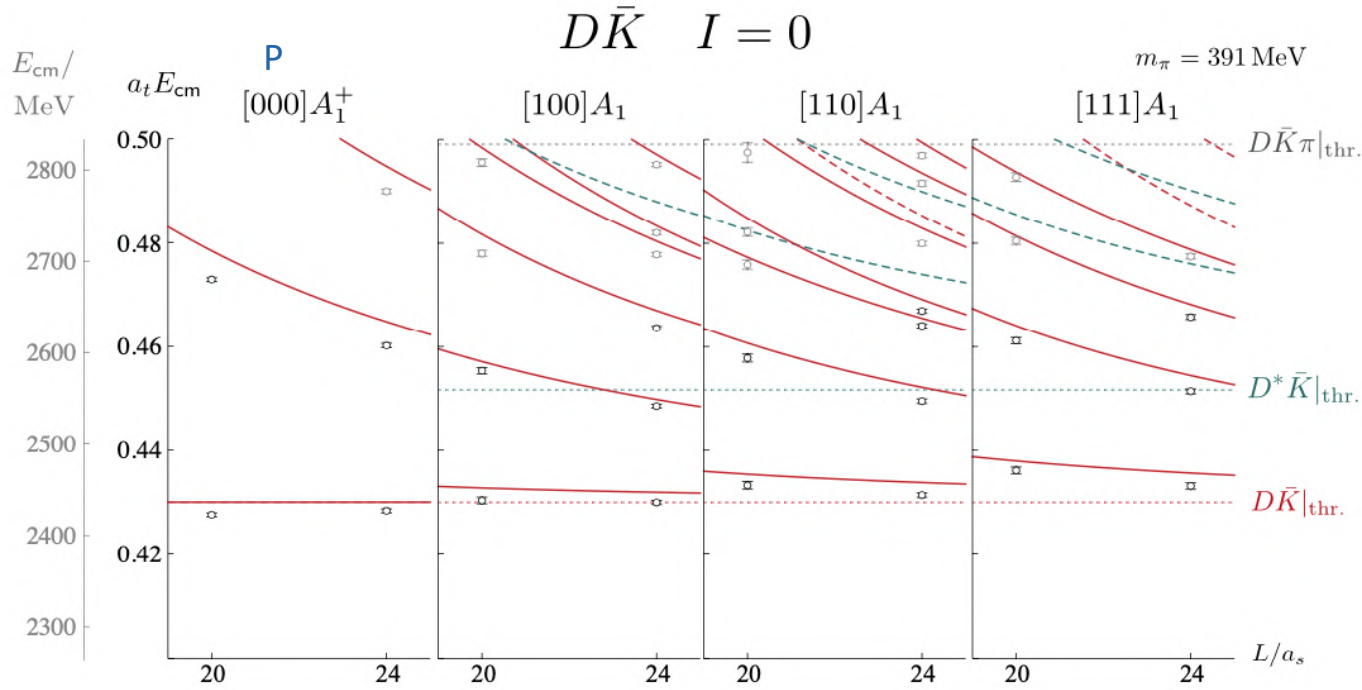
$$p \cot \delta(p) = \frac{1}{a_0} + \frac{1}{2}r_0 p^2$$

$D^- K^+$

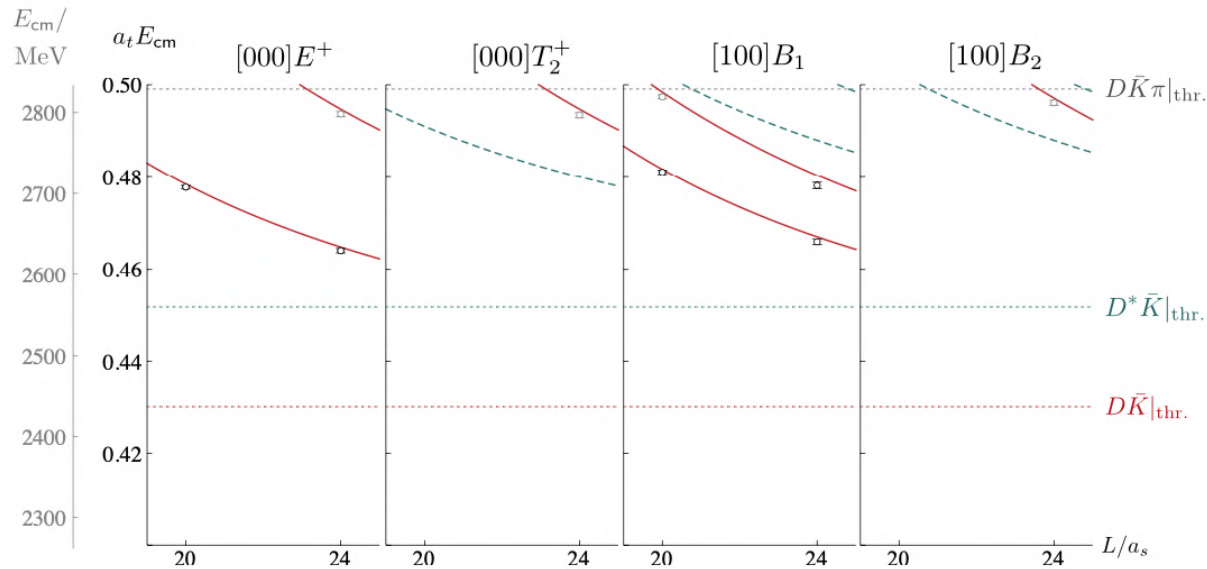
$\bar{c}d \bar{s}u$

explicitly exotic flavor

HadSpec. Coll, 2008.06432

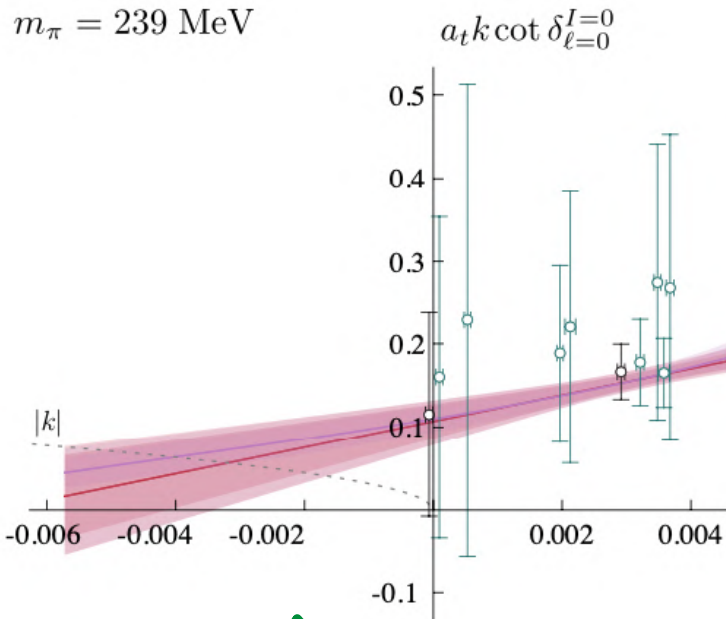


certain irrep gets  
contribution from multiple  
partial waves (odd and even)  
for  $P \neq 0$  since  $m_D \neq m_K$



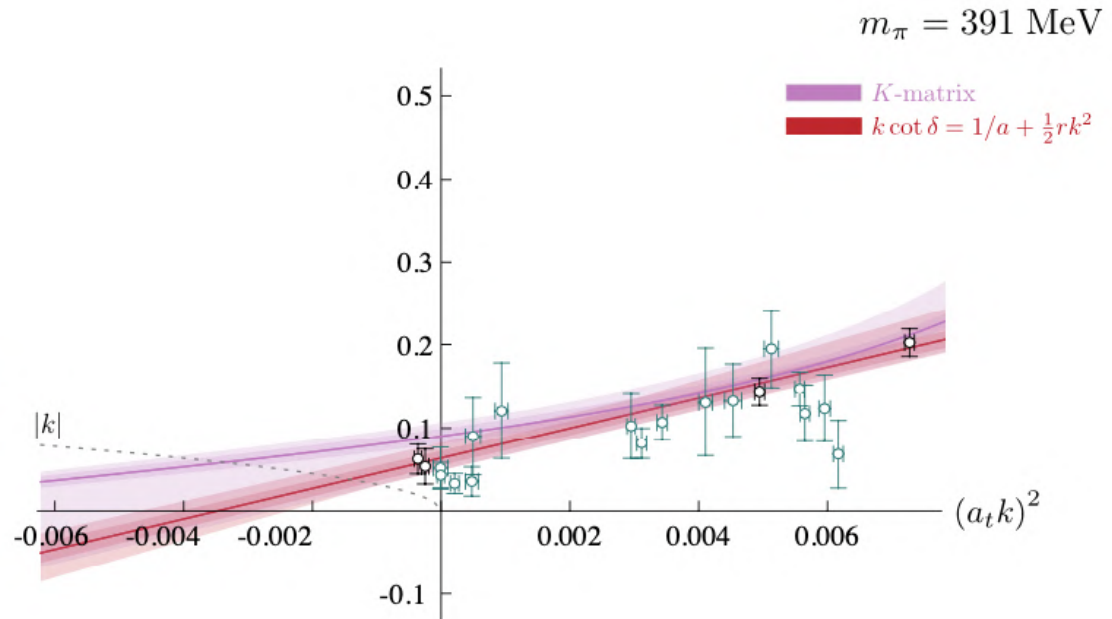
# $D^- K^+, J^P=0^+, I=0$

$m_\pi = 239$  MeV



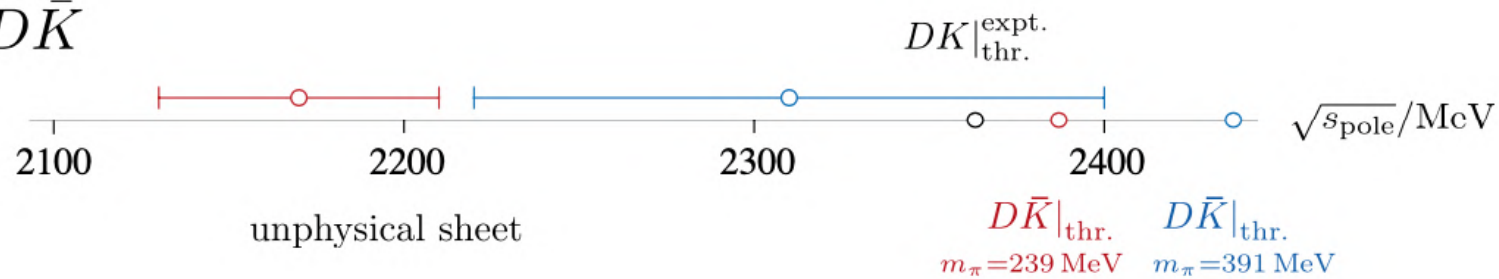
$VB \uparrow$

$m_\pi = 391$  MeV



$VB \uparrow$

$D\bar{K}$





$D^- K^+$ 

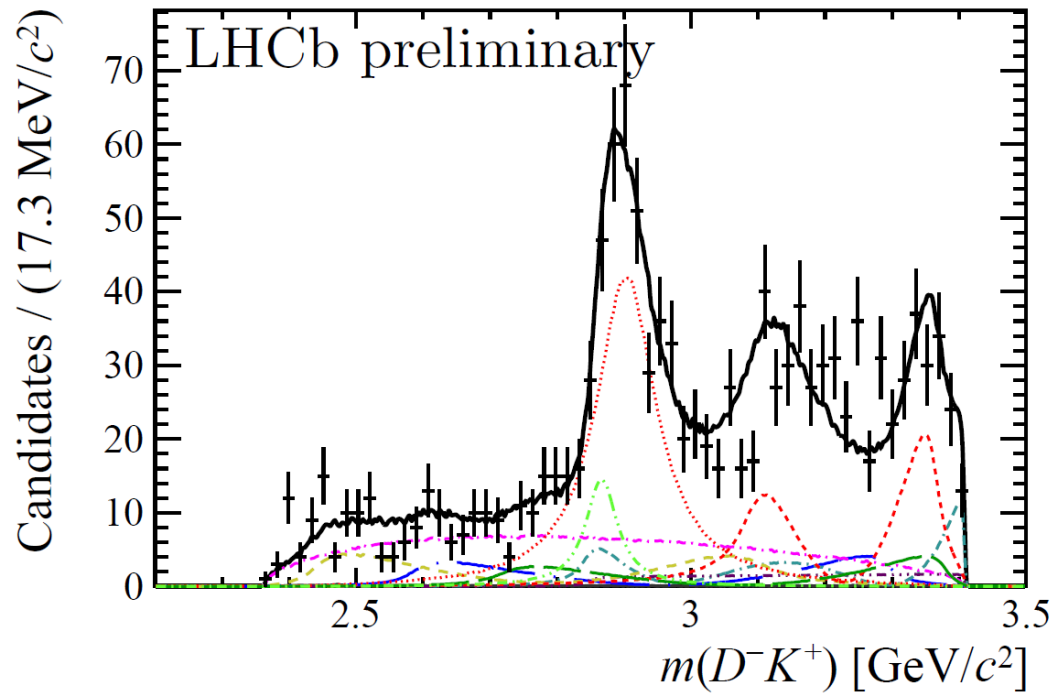
exp evidence for two exotic resonances

LHCb

2009.00025, 2009.00026

 $\bar{c}d \bar{s}u$ 

explicitly exotic flavor, isospin from exp: 0 or 1 ?



- .....  $\psi(3770) \rightarrow D^+ D^-$
- .....  $\chi_{c0}(3930) \rightarrow D^+ D^-$
- .....  $\chi_{c2}(3930) \rightarrow D^+ D^-$
- .....  $\psi(4040) \rightarrow D^+ D^-$
- .....  $\psi(4160) \rightarrow D^+ D^-$
- .....  $\psi(4415) \rightarrow D^+ D^-$
- .....  $X_0(2900) \rightarrow D^- K^+$
- .....  $X_1(2900) \rightarrow D^- K^+$
- ..... Nonresonant

Resonance	Mass (GeV/c <sup>2</sup> )	Width (MeV)
$X_0(2900)$	$2.866 \pm 0.007 \pm 0.002$	$57 \pm 12 \pm 4$
$X_1(2900)$	$2.904 \pm 0.005 \pm 0.001$	$110 \pm 11 \pm 4$

near  $D^*K^*$  thr.energy  $E_{\text{cm}} = 2.9 \text{ GeV}$ 

not reached by HSC lattice sim.