Few-body Systems in Physics Laboratory
RNC, RIKEN

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Tetraquark states in the Diffusion Monte Carlo method

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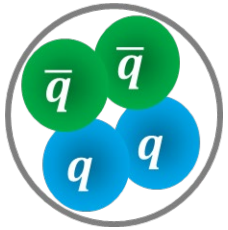
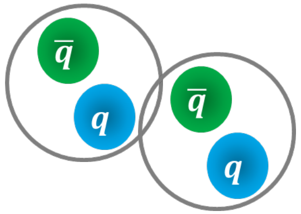
12th July, 2023

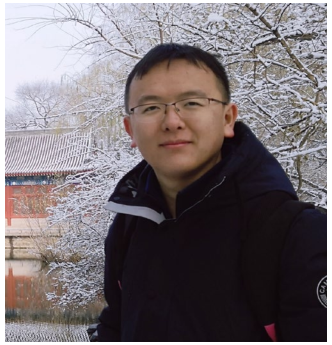


Based on PRD107(2023),054035 and papers in preparation

Together with Yan-Ke Chen, Yao Ma and Shi-Lin Zhu (PKU)



- Background
- Gaussian expansion method
- Resonating group method


Lu Meng


Yao Ma


Yan-Ke Chen

- **Diffusion Monte Carlo Method**

- Summary

History of the multiquark states

Phys.Lett. 8 (1964) 214-215

Volume 8, number 3 PHYSICS LETTERS 1 February 1964

A SCHEMATIC MODEL OF BARYONS AND MESONS *

M. GELL-MANN
California Institute of Technology, Pasadena, California

Received 4 January 1964

. . .

A simpler and more elegant scheme can be constructed if we allow non-integral values for the charges. We can dispense entirely with the basic baryon b if we assign to the triplet t the following properties: spin $\frac{1}{2}$, $z = -\frac{1}{3}$, and baryon number $\frac{1}{3}$. We then refer to the members $u^{\frac{2}{3}}$, $d^{-\frac{1}{3}}$, and $s^{-\frac{1}{3}}$ of the triplet as "quarks" 6) q and the members of the anti-triplet as anti-quarks $\bar{q}$. Baryons can now be constructed from quarks by using the combinations $(q\,q\,q)$, $(q\,q\,q\,q\,\bar{q})$, etc., while mesons are made out of $(q\,\bar{q})$, $(q\,q\,\bar{q}\,\bar{q})$, etc. It is assuming that the lowest baryon configuration $(q\,q\,q)$ gives just the represen-

8419/TH.412
21 February 1964

AN SU_3 MODEL FOR STRONG INTERACTION SYMMETRY AND ITS BREAKING

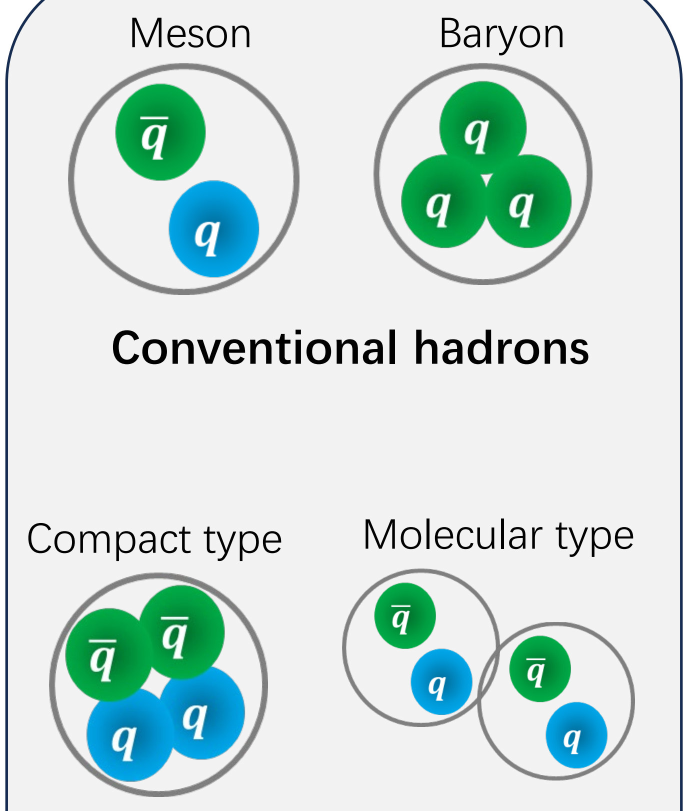
II *)

G. Zweig
CERN---Geneva

*) Version I is CERN preprint 8182/TH.401, Jan. 17, 1964.

. . .

6) In general, we would expect that baryons are built not only from the product of three aces, AAA, but also from $\overline{A}$AAAA, $\overline{AA}$AAAAA, etc., where $\overline{A}$ denotes an anti-ace. Similarly, mesons could be formed from $\overline{A}$A, $\overline{AA}$AA etc. For the low mass mesons and baryons we will assume the simplest possibilities, $\overline{A}$A and AAA, that is, "deuces and treys".

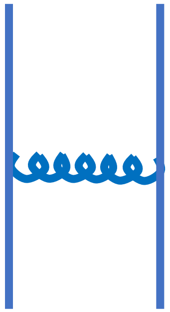


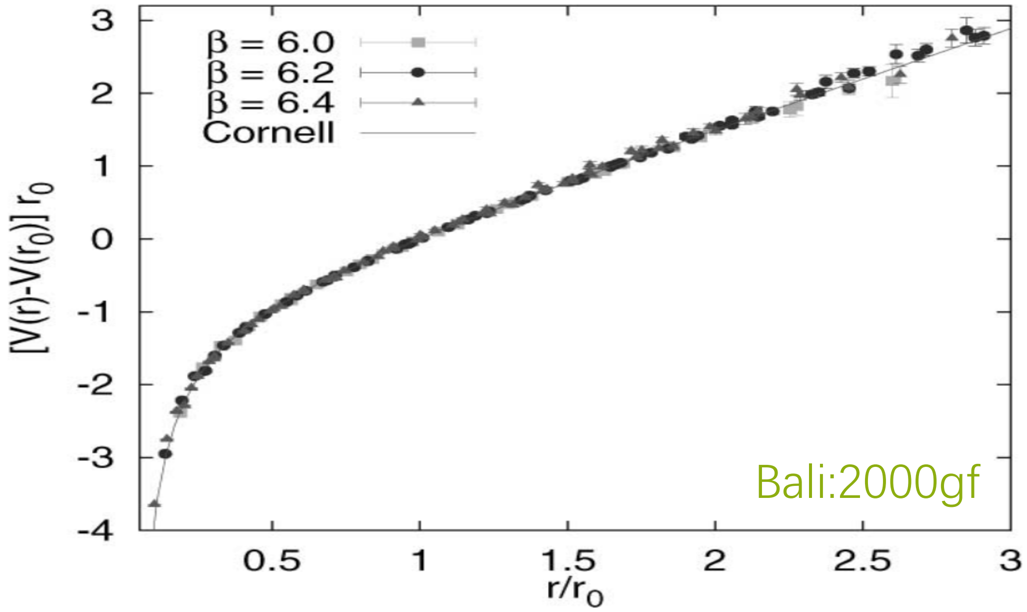
- The multiquark states were predicted at the birth of Quark model

Quark potential models

- A minimal model: one-gluon-exchange+Confinement   Eichten:1978tg, Barnes:2005pb⋯

$$V_{ij}(r) = \left[\underbrace{\frac{\alpha_s}{r} - \frac{8\pi\alpha_s}{3m_i m_j}\frac{\tau^3}{\pi^{3/2}}e^{-\tau^2 r^2}\boldsymbol{s}_i\cdot\boldsymbol{s}_j}_{\text{OGE}} + \underbrace{\left(-\frac{3b}{4}r + V_c\right)}_{\text{Confinement}}\right]\frac{\lambda_i\cdot\lambda_j}{4}$$

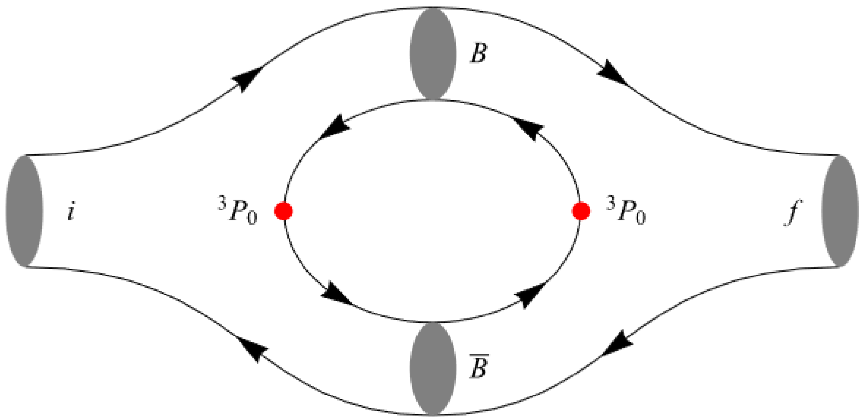




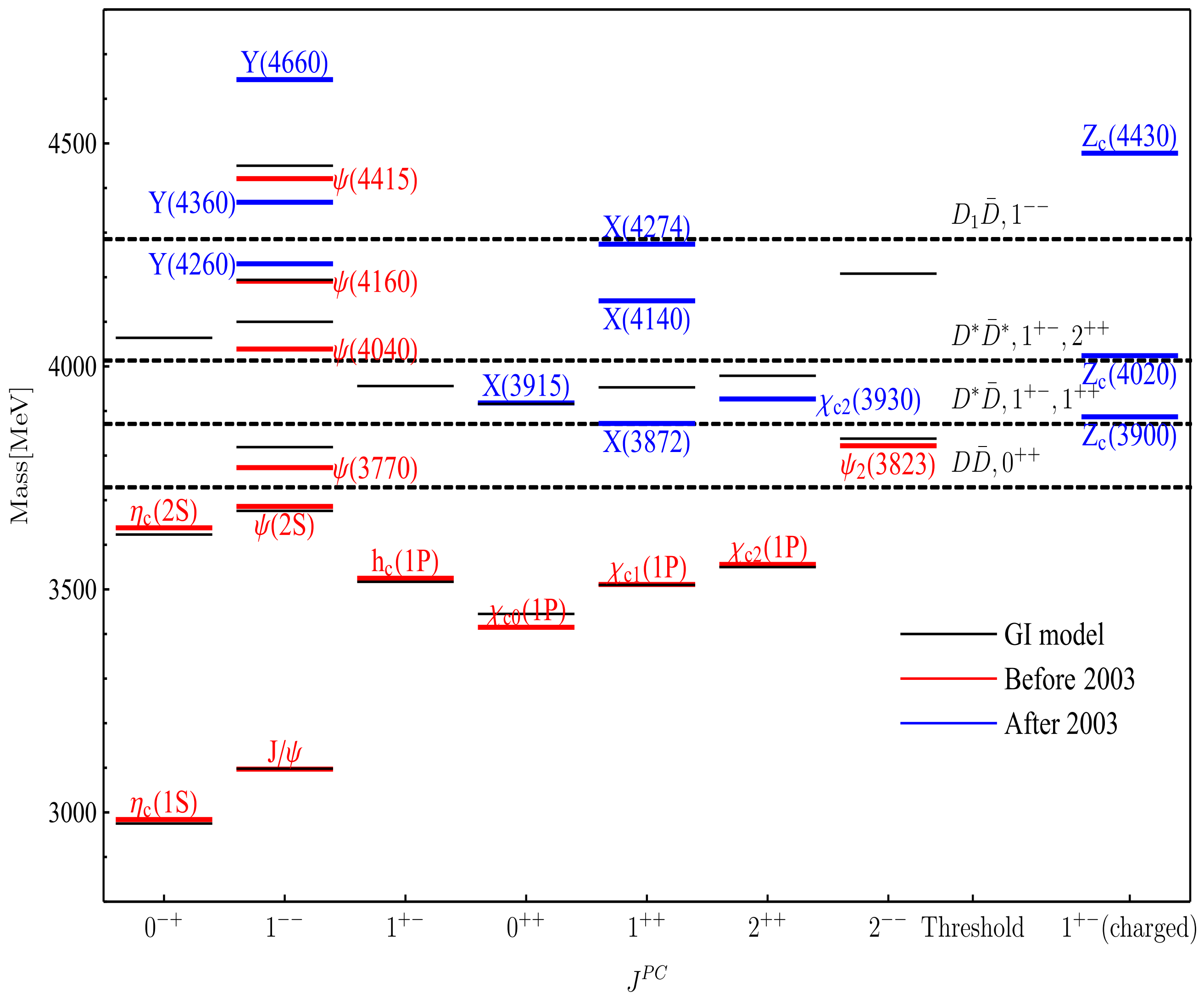
- Relativized Godfrey-Isgur model   Godfrey:1985xj

Tetraquark states

- Since 2003, many heavy-quarkonium-like states were observed.
  - ► Hard to include them in the patten predicted by quark models
  - ► Most of them are above the di-meson thresholds
- The unquenched effect



- Ones with exotic quantum numbers are tetraquark states without doubt
  - ► $Z_c(3900)$, $Z_c(4020)$



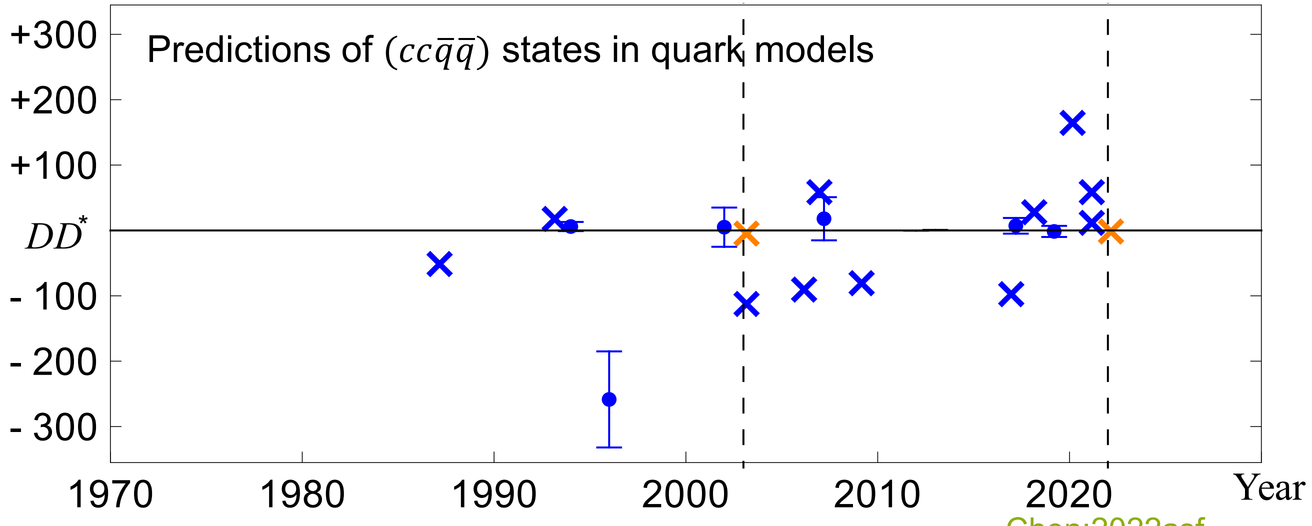
Tetraquark states

- Recently, more and more hadrons composed of at least four quarks were observed

New naming scheme: Gershon:2022xnn

$[c\bar{c}qqq]$ P_c	$[cc\bar{c}\,\bar{c}]$ $X(6900)$	$[cs\bar{u}\,\bar{d}]$ $T_{cs1}(2900)$ $T_{cs0}(2900)$	$[cs\bar{u}\,\bar{d}]$ $Z_{cs}(3985)$ $Z_{cs}(4000)$	$[cc\bar{u}\,\bar{d}]$ $T_{cc}(3875)^+$	$[c\bar{s}u\bar{d}][c\bar{s}\bar{u}d]$ $T_{c\bar{s}0}(2900)^{++}$ $T_{c\bar{s}0}(2900)^0$
	2006.16957 2304.08962 …	2009.00025 2009.00026	2011.07855 2103.01803	2109.01038 2109.01056	2212.02716 2212.02717

- Different quark models predicted different results
  - ▶ Example: T_{cc} states



Chen:2022asf

- What is responsible for variations?

InteractionS + few-body methodS

- Benchmark calculations

(AL1,AP1,SLM)⊗(GEM,RGM,DMC)

Benchmark test calculation of a four-nucleon bound states

Benchmark Test Calculation of a Four-Nucleon Bound State

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Method	E_b
Faddeev-Yakubovsky Eq.	-25.94(5)
Gaussian basis expansion	-25.90
stochastic variational method	-25.92
Hyperspherical variational	-25.90(1)
Green's function MC/Diffusion MC	-25.93(2)
No-core shell model	-25.80(20)
Hyperspherical harmonic methods	-25.944(10)

Kamada:2001tv

Quark potential models

- Semay-Silvestre-Brac Models

Semay:1994ht, Silvestre-Brac:1996myf

$$V_{ij}(r) = \left[-\frac{\kappa}{r} + \lambda r^p - \Lambda + \frac{2\pi}{3m_i m_j}\kappa' \frac{1}{\pi^{3/2} r_0^3} e^{(-r^2/r_0^2)} \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j \right] \lambda_i \cdot \lambda_j$$

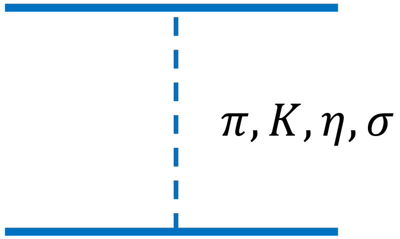
AL1: $p = 1$ and AP1: $p = 2/3$

- Chiral quark models [e.g Salamanca model (SLM)]

Vijande:2004he, Gonzalez:2012gka

$$V_{ij}(r) = \left[\frac{\alpha_s}{4} \left(\frac{1}{r} - \frac{1}{6m_i m_j} \frac{e^{-r/r_0}}{r_0^2 r} \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j \right) + \underbrace{\left(-a_c (1 - e^{-\mu_c r}) + \Delta \right)}_{\text{Screened confinement}} \right] \lambda_i \cdot \lambda_j$$

$$+V_\pi + V_K + V_\eta + V_\sigma$$



- In this work, we use AL1, AP1 and SLM

[GeV]	π	K	D	D_s	B	B_s	B_c	η_c	η_b
Exp.	0.139	0.494	1.870	1.968	5.279	5.367	6.274	2.984	9.399
AL1	0.138	0.491	1.862	1.962	5.293	5.361	6.292	3.005	9.424
AP1	0.139	0.498	1.881	1.955	5.311	5.356	6.269	2.982	9.401
SLM	0.140	0.469	1.896	1.983	5.275	5.348	6.275	2.990	9.451

Quark potential models

- Semay-Silvestre-Brac Models

Semay:1994ht, Silvestre-Brac:1996myf

$$V_{ij}(r) = \left[-\frac{\kappa}{r} + \lambda r^p - \Lambda + \frac{2\pi}{3m_i m_j}\kappa' \frac{1}{\pi^{3/2} r_0^3} e^{(-r^2/r_0^2)} \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j \right] \lambda_i \cdot \lambda_j$$

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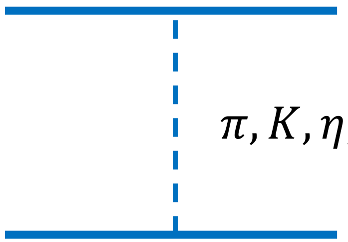
$$+V_\pi + V_K + V_\eta + V_\sigma$$



- In this work, we use AL1, AP1 and SLM

[GeV]	ρ	ω	ϕ	K^*	D^*	D_s^*	B^*	B_s^*	B_c^*	J/ψ	Υ
Exp.	0.775	0.783	1.019	0.892	2.010	2.112	5.325	5.415	6.329	3.097	9.460
AL1	0.770	0.770	1.021	0.903	2.016	2.102	5.350	5.417	6.343	3.101	9.461
AP1	0.770	0.770	1.021	0.908	2.033	2.107	5.367	5.418	6.338	3.102	9.461
SLM	0.773	0.693	1.000	0.902	2.018	2.111	5.317	5.393	6.329	3.097	9.501

Gaussian Expansion Method

Gaussian Expansion Method

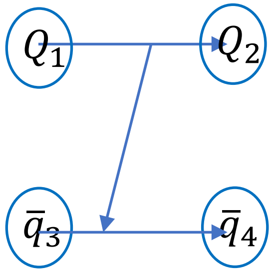
- Color functions

$$\begin{cases}[(Q_1Q_2)_{\bar{3}}(\bar{q}_3\bar{q}_4)_3]_1\\ [(Q_1Q_2)_6(\bar{q}_3\bar{q}_4)_{\bar{6}}]_1\end{cases} \quad \text{Or} \quad \begin{cases}[(Q_1\bar{q}_3)_1(Q_2\bar{q}_4)_1]_1\\ [(Q_1\bar{q}_4)_1(Q_2\bar{q}_3)_1]_1\end{cases} \quad \text{Or} \quad \begin{cases}[(Q_1\bar{q}_3)_1(Q_2\bar{q}_4)_1]_1\\ [(Q_1\bar{q}_4)_8(Q_2\bar{q}_3)_8]_1\end{cases}$$

- Spin wave function

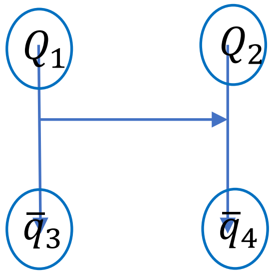
$$S_{12} = 0,1;\ S_{34} = 0,1 \quad S_{12}\otimes S_{34}\to J \qquad \text{Or} \qquad S_{13} = 0,1;\ S_{24} = 0,1 \quad S_{13}\otimes S_{24}\to J \qquad \text{Or} \qquad S_{14} = 0,1;\ S_{23} = 0,1 \quad S_{14}\otimes S_{23}\to J$$

- Spatial wave functions



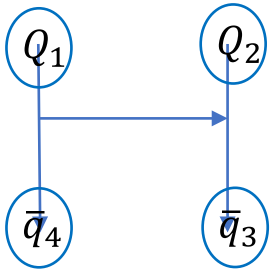
Diquark-antidiquark

And



Di-meson

And



Di-meson

$$\phi_{nlm}(\boldsymbol{r}) = N_{lm} r^l e^{-\frac{r^2}{r_n^2}} Y_{lm}(\hat{r})$$

Geometric progression

$r_n = r_0 a^{n-1}$

Hiyama:2003cu

Embed both long- and short-range correlations

- Antisymmetrization (e.g. $Q_1 = Q_2$ and $q_3 = q_4$) :

$$\psi = \mathcal{A}[\psi_{color}\otimes\psi_{spin}\otimes\psi_{spatial}\otimes\psi_{flavor}], \qquad \mathcal{A} = (1-P_{12})(1-P_{34})$$

Tetraquark systems

- Fully heavy tetraquark states ($QQ\bar{Q}\bar{Q}$)
- Triply heavy tetraquark states ($QQ\bar{Q}\bar{q}$)
- Doubly heavy tetraquarks states ($QQ\bar{q}\bar{q}$)
- Single heavy strange states ($Qs\bar{q}\bar{q}$, $Q\bar{s}q\bar{q}$)

$q = u, d, s;\ \ Q = b, c$

- $J^P = 0^+, 1^+, 2^+$
  - ▶ Only S-wave

Over 150 states

- In this work, we only focus on bound states

Wang:2019rdo, Meng:2021yjr⋯

	$QQ\bar{Q}\bar{Q}$	$QQ\bar{Q}\bar{q}$	$QQ\bar{q}\bar{q}$	$Qs\bar{q}\bar{q}$	$Q\bar{s}q\bar{q}$
$J^P = 0^+$	No bound	No bound	😊	😊	No bound
$J^P = 1^+$	No bound	No bound	😊	😊	No bound
$J^P = 2^+$	No bound	No bound	😊	😊	No bound

- Masses are shifted to align the theoretical thresholds with the physical ones.

$QQ\bar{q}\,\bar{q}$ with $J^P = 1^+$

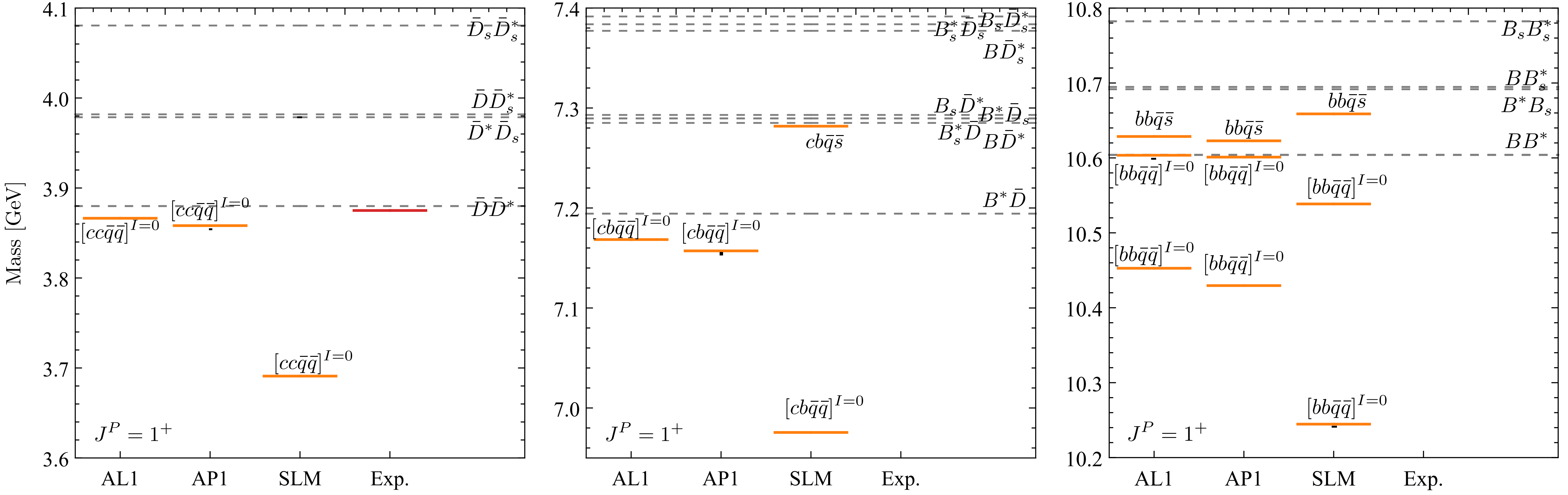
Preliminary

- Points of agreement
  - ► $[QQ\bar{q}\,\bar{q}]^{I=0}$ ($QQ = cc$ or bb or bc) bound states ; $[bb\bar{q}\bar{s}]$ bound states
  - ► For $[bb\bar{q}\,\bar{q}]^{I=0}$ systems, the 1st excited states are bound states
  - ► No $[QQ\bar{q}\,\bar{q}]^{I=1}$ states

Different with that in Ortega:2022efc

- SLM

  (1) $[cc\bar{q}\bar{q}]^{I=0}$ are too deep compared with ex. (200MeV VS 200 keV); (2) $[cb\bar{q}\bar{s}]$ bound states



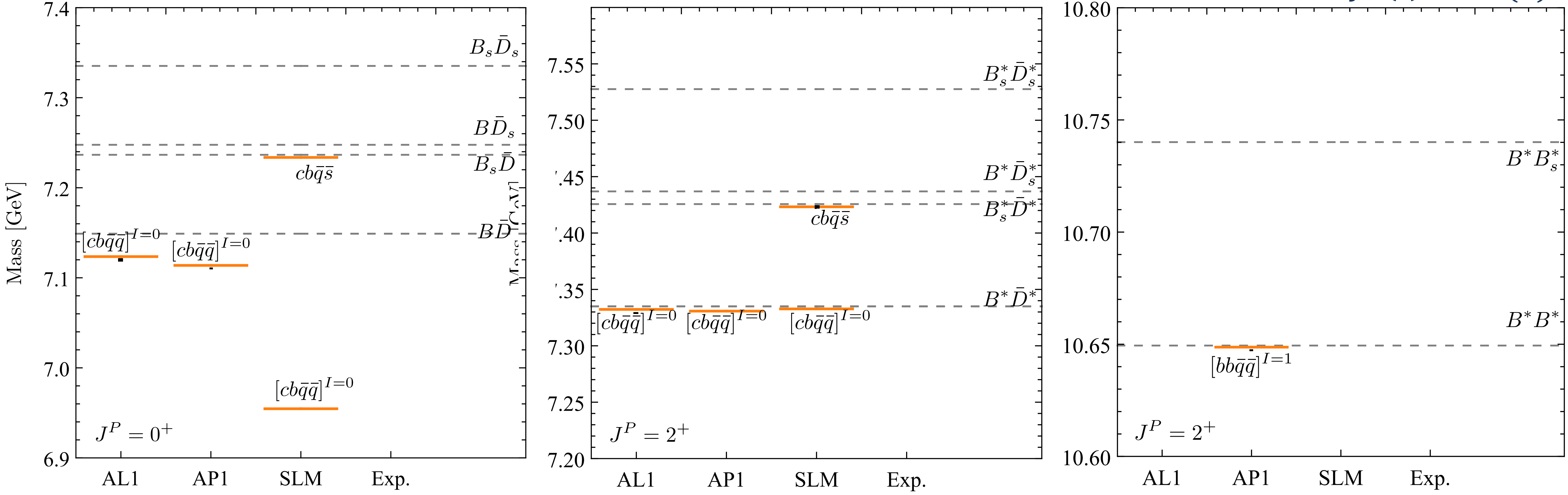
$QQ\bar{q}\,\bar{q}$ with $J^P = 0^+, 2^+$

- Points of agreement
  - ▶ $[cb\bar{q}\,\bar{q}]^{I=0}$ bound states for $J^P = 0^+, 2^+$
- SLM: $cb\bar{q}\bar{s}$ bound states for $J^P = 0^+, 2^+$
- AP1: $bb\bar{q}\bar{s}$ bound states for $J^P = 2^+$

TABLE VII. Properties of the T_{bb} candidates as $B^{(*)}B^{(*)}$ molecules in the $J^P = 0^+$ and 2^+ sectors obtained in this work. Masses, widths, binding energies and partial widths are shown in MeV/c^2. Ortega:2022efc

J^P	I	Mass	Width	E_B	$\mathcal{P}_{BB}$	$\mathcal{P}_{B^*B^*}$	Γ_{BB}	$\Gamma_{B^*B^*}$
0^+	0	10553.0	0	6.0	92%	8%	0	0
		10640.7	2.8	8.7	76%	24%	2.8	0
	1	10545.9	0	13.1	93%	7%	0	0
		10672.6	72.0	−23.2	39%	61%	30.7	41.3
2^+	1	10642.3	0	7.1	-	100%	-	0

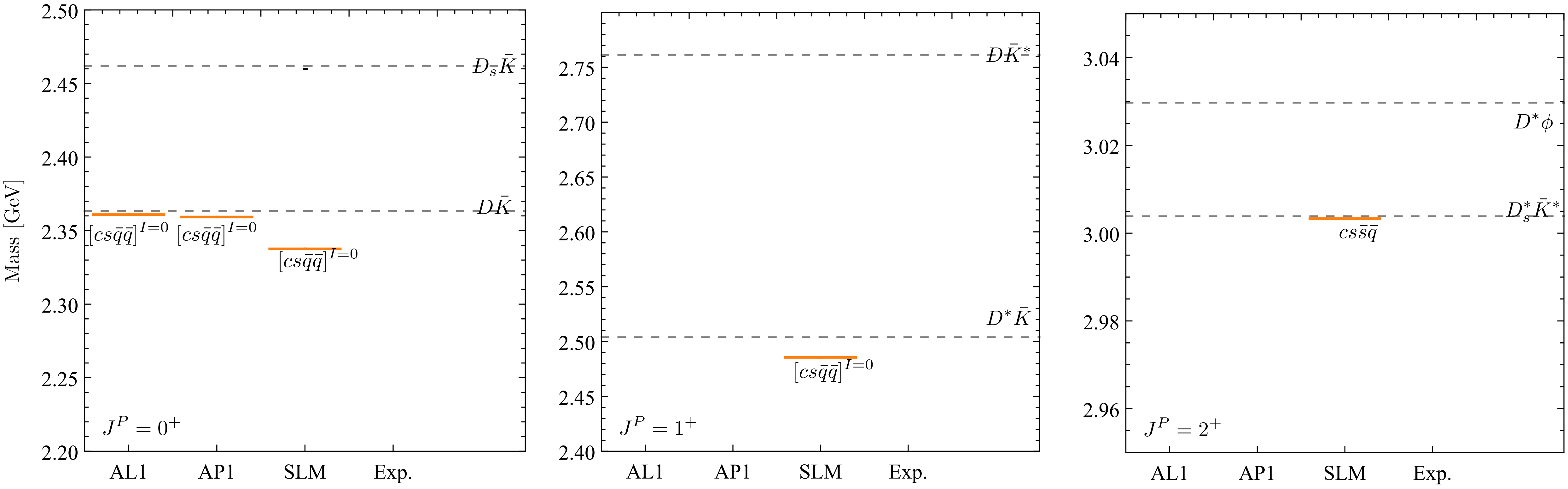
The S-wave BB states can not be $J^P(I) = 0^+(0)$



$cs\bar{q}\bar{q}$ systems with $J^P = 0^+, 1^+, 2^+$

- Points of agreement
  - ▶ $[cs\bar{q}\,\bar{q}]^{I=0}$ bound states for $J^P = 0^+$
- SLM:
  - ▶ $[cs\bar{q}\bar{q}]^{I=0}$ for $J^P = 1^+$and $cs\bar{s}\bar{q}$ for $J^P = 2^+$ bound states
- Note: The experimental $T_{cs0}(2900)$ and $T_{cs1}(2900)$ are close to $D^*\bar{K}^*$ thresholds, resonances

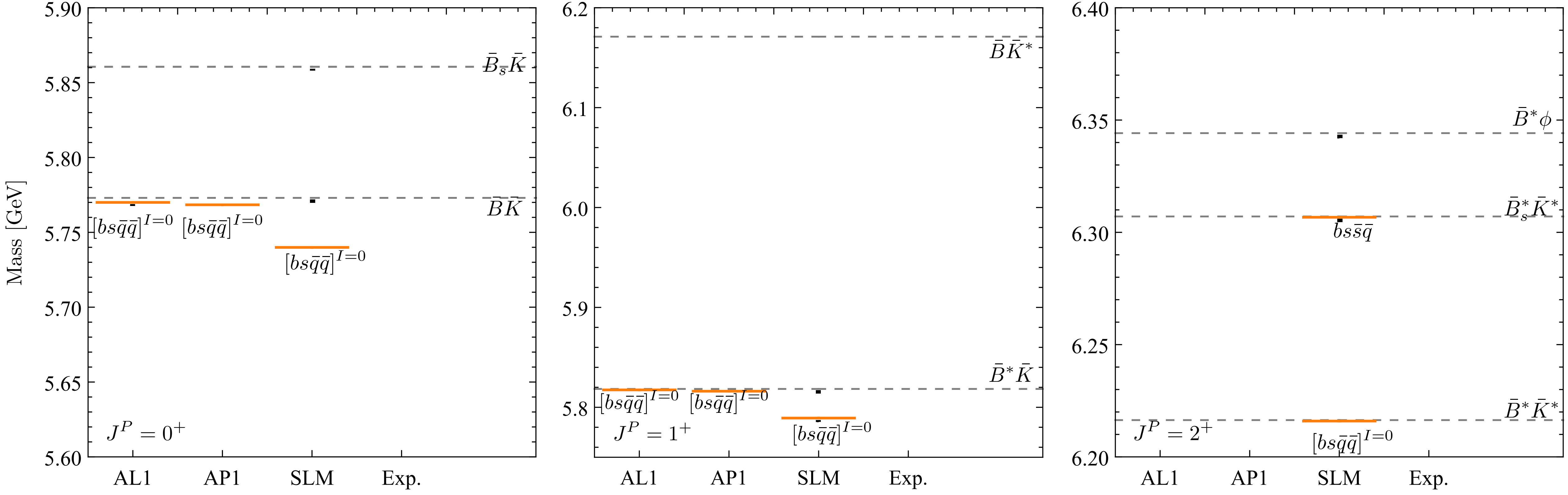
Preliminary



$bs\bar{q}\bar{q}$ systems with $J^P = 0^+, 1^+, 2^+$

- Points of agreement
  - ▶ $[bs\bar{q}\,\bar{q}]^{I=0}$ bound states for $J^P = 0^+, 1^+$
- SLM:
  - ▶ $[bs\bar{q}\bar{q}]^{I=0}$ and $bs\bar{s}\bar{q}$ for $J^P = 2^+$ bound states

SLM tends to predict extra states



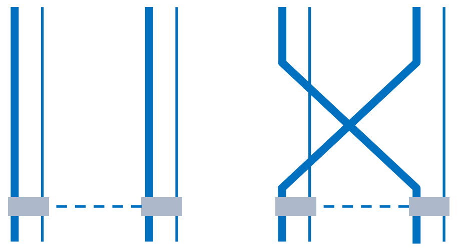
Resonating Group Method

Resonating Group Method

- Dimeson-wave function

$$\psi_{AB}(\boldsymbol{P}) = \mathcal{A}[\phi_A(\boldsymbol{p}_A)\phi_B(\boldsymbol{p}_B)\chi(\boldsymbol{P})\chi_{AB}^{CST}]$$

  - ▶ ϕ_A and ϕ_B are meson wave functions
  - ▶ We use GEM to get the meson wave functions
  - ▶ $\mathcal{A}$ represents antisymmetriziation operator of identical quarks



Entem:2000mq, Ortega:2022efc

- Schrodinger equation of RGM

$$\left(\frac{\boldsymbol{P}'^2}{2\mu} - E\right)\chi(\boldsymbol{P}') + \int d^3\boldsymbol{P}\,(V_D(\boldsymbol{P}',\boldsymbol{P}) + K_{Ex}(\boldsymbol{P}',\boldsymbol{P}))\,\chi(\boldsymbol{P}) = 0$$

  - ▶ V_D direct interaction, K_{Ex} the exchange kernel

- Compared with GEM
  - ▶ The spin-color-flavor wave functions are complete as well
  - ▶ The RGM neglecting the distortion of the meson wave functions in the tetraquark system
  - ▶ Only the di-meson-type spatial correlations are included
  - ▶ The trial functions are not as general as GEM

$$E_{RGM} \gtrsim E_{GEM}$$

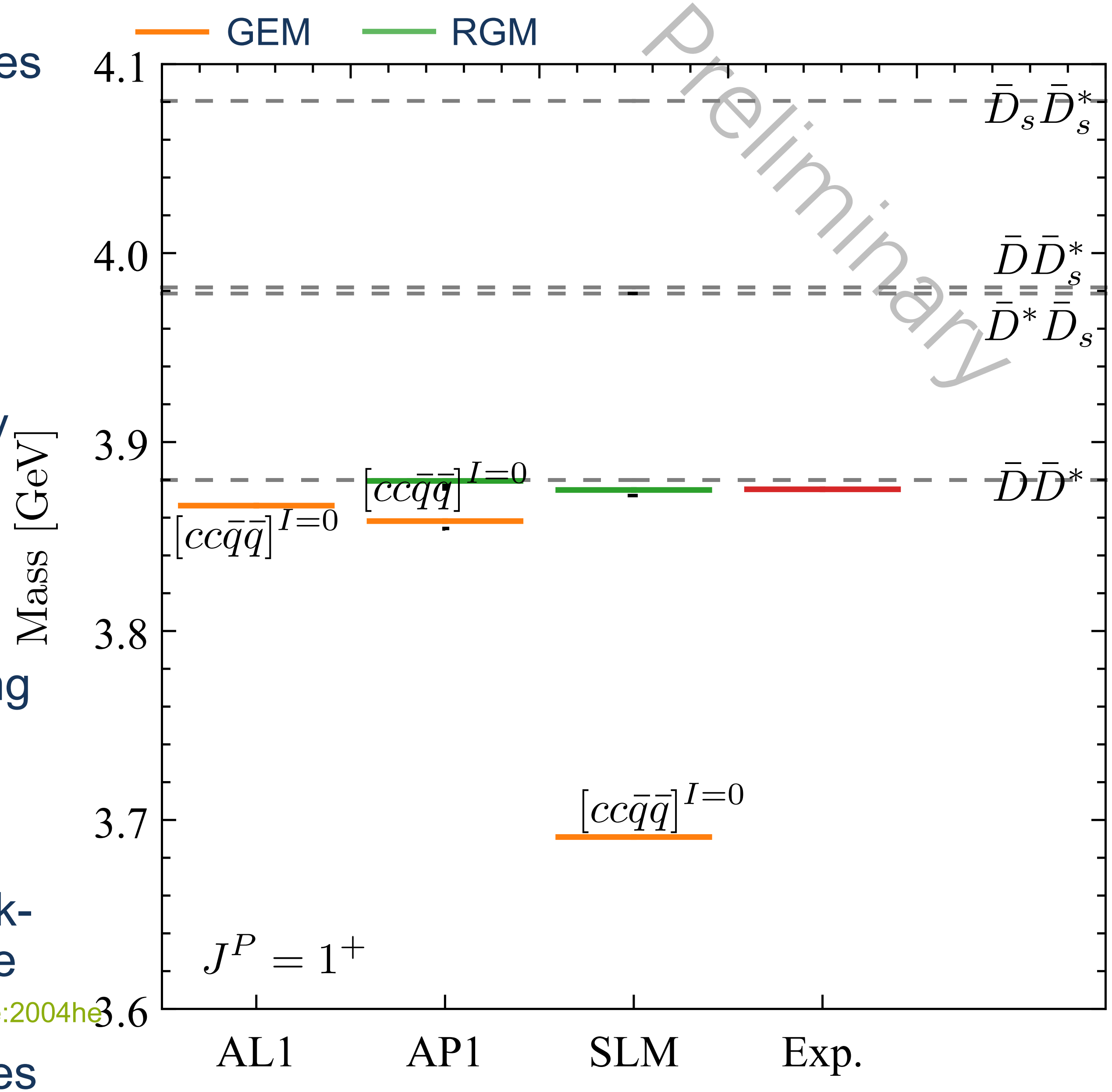
RGM results

- The RGM gives the smaller binding energies
  - ▶ Without the diquark-antidiquark-type correlation
- The RGM results agree with the GEM neglecting diquark-antidiquark correlation
  - ▶ Not general enough trail wave function
  - ▶ Cannot get the ground state accurately
  - ▶ A drawback as a few-body method

However…

- Some quark models (e.g. SLM) constraining the para. using NN phase shifts with RGM
  - ▶ The spatial correlations other than di-hadron types are neglected from birth
  - ▶ Perhaps, it is misleading to use diquark-antidiquark type trial functions for these models
  - ▶ Otherwise, deeper or extra bound states

Entem:2000mq, Vijande:2004he



RGM results

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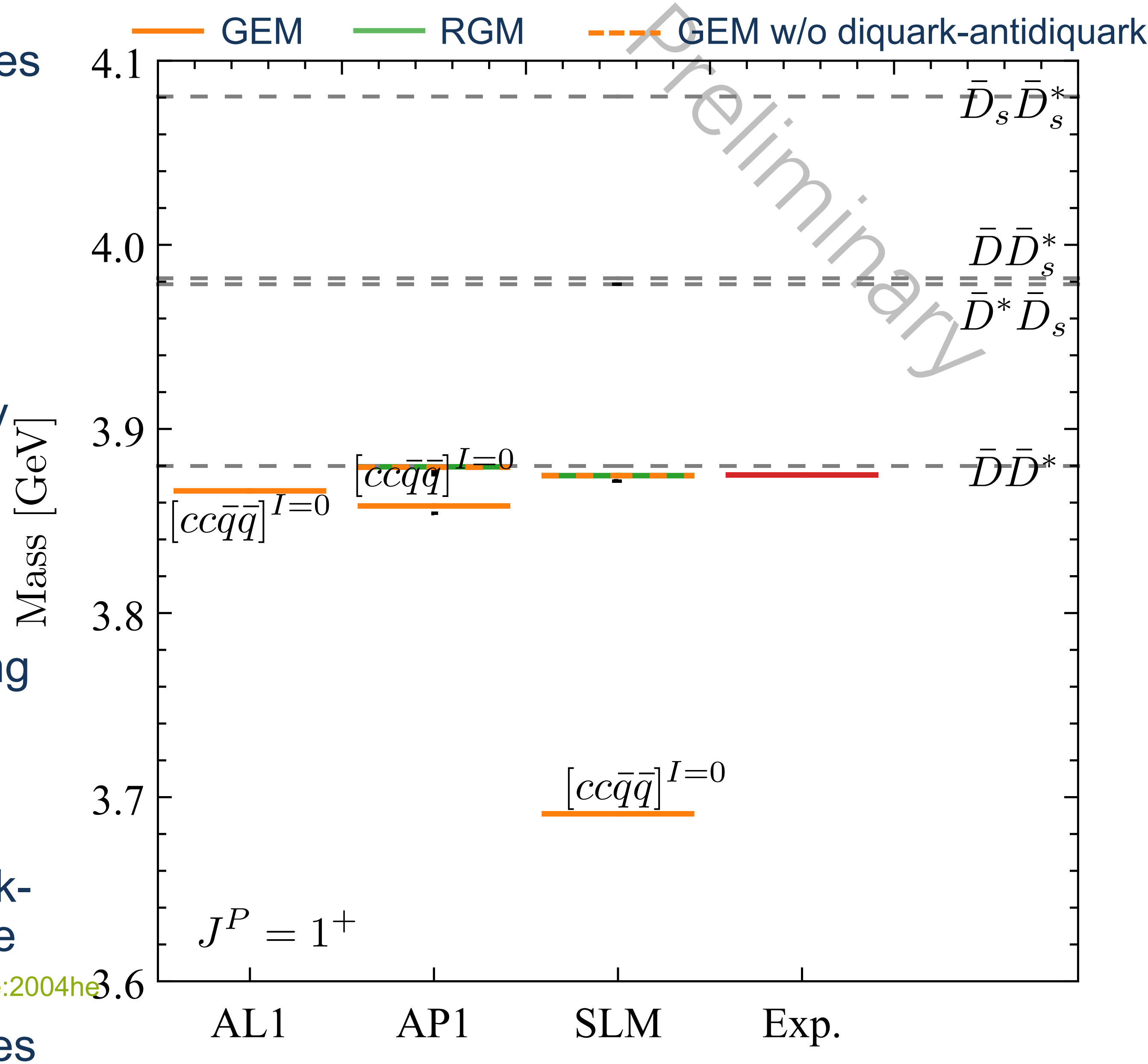
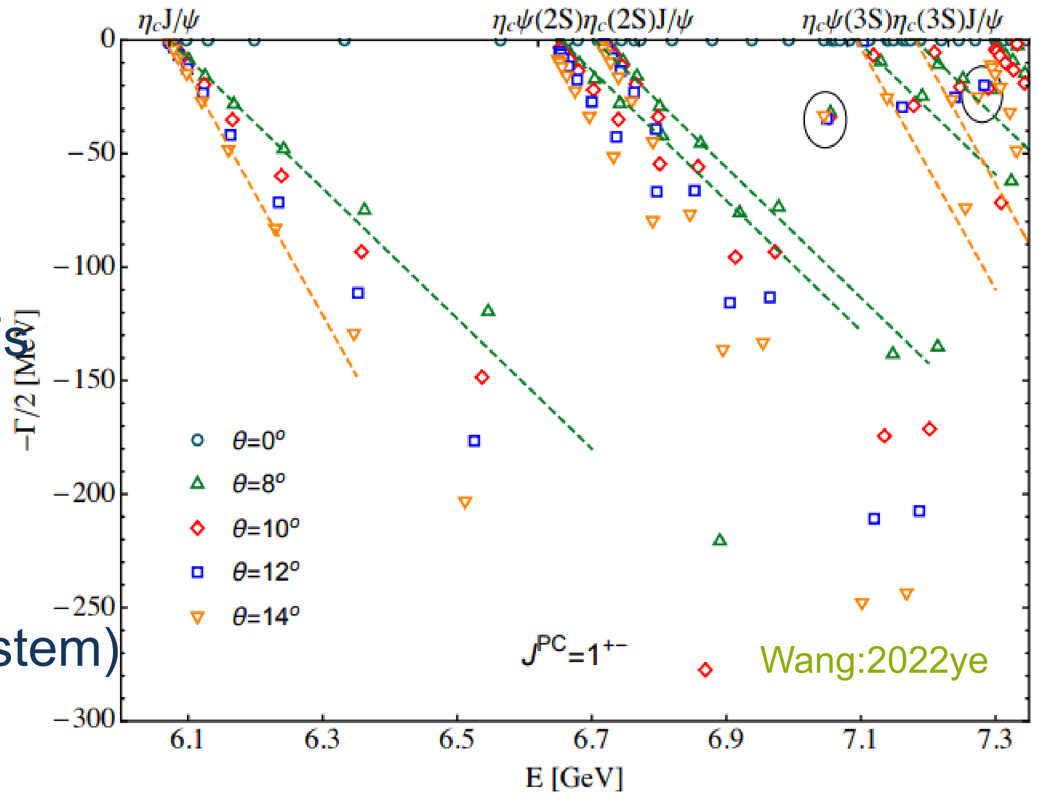


RGM: promising method for tetraquark resonance

- Due to the color confinements, some thresholds make no sense
  - ▶ The four quark threshold $(q)(q)(\bar{q})(\bar{q})$
  - ▶ The $(qq\bar{q})(q)$, $(\bar{q}\bar{q}q)$ (q) thresholds
  - ▶ The diquark-antidiquark threshold $(qq)(\bar{q}\bar{q})$

- For continuum, only the di-mesons are relevant D.O.Fs

- RGM in p-space:
  - ▶ Coupled-channel two-body scattering
  - ▶ Simpler Riemann sheet structure (than 4-body system)



- Slove the RGM in p-space
  - ▶ LSE + Inverse matrix method Entem:2000mq, Ortega:2022efc
  - ▶ Schrodinger Eq. + Generalized Complex Scaling method Lin:2022wmj, Lin:2023dbp, and work in preparation

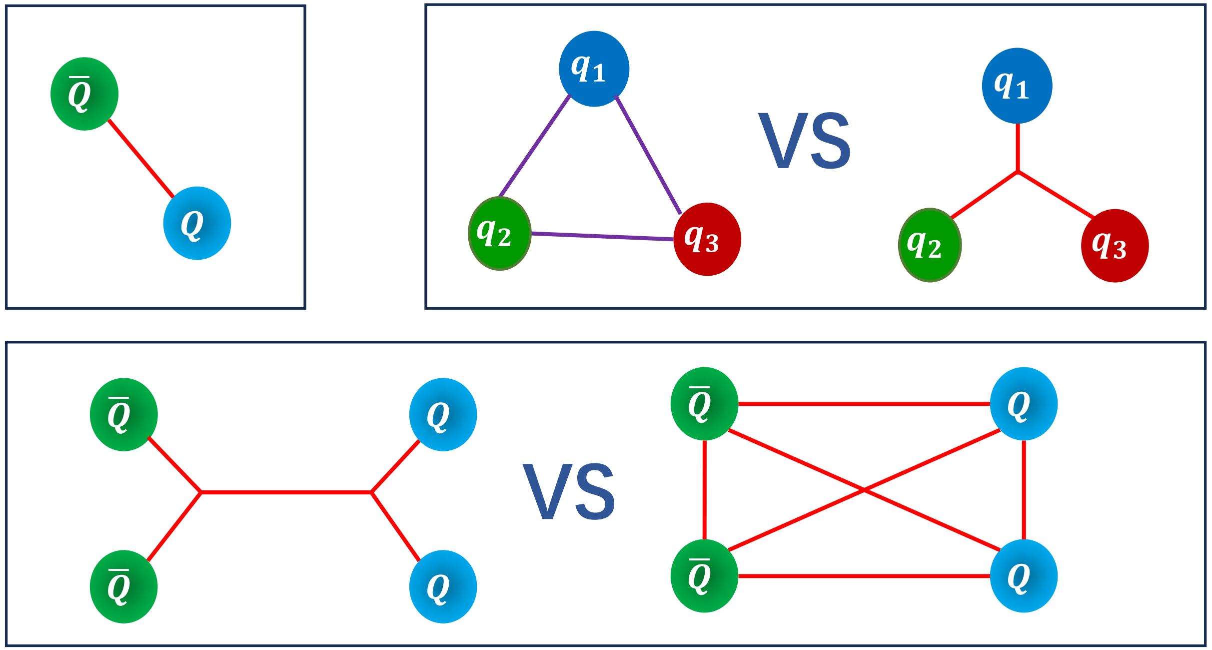
  Solving Fredholm determinant⇒ Eigenvalue problem

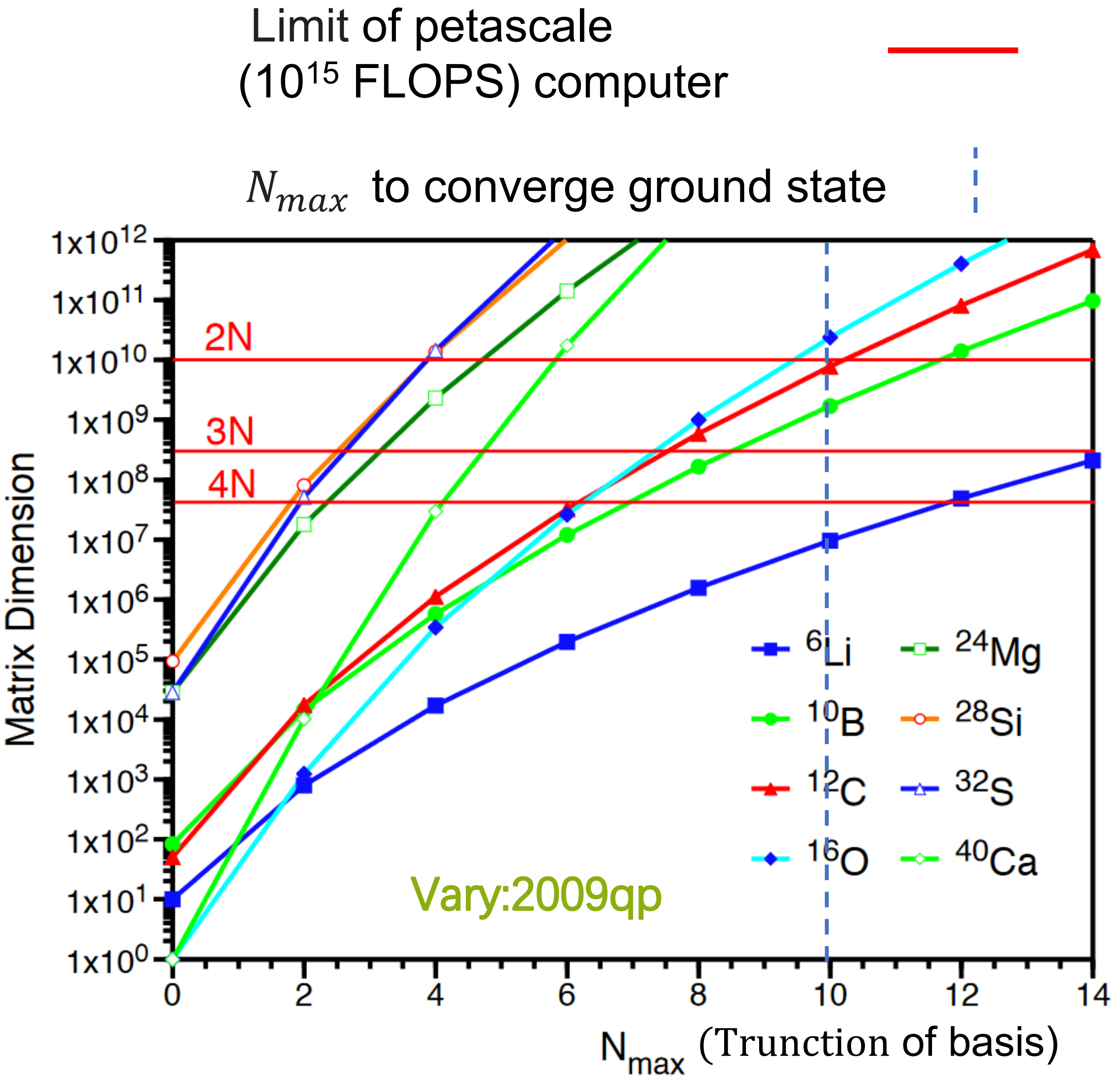
Diffusion Monte Carlo method

Motivations

- The computational cost of variational methods increases exponentially with N
  - ▶ Computational cost of No-core-shell-model
  - ▶ A variational method using HO basis
- The three-body and four-body force
- Confinement mechanisms in multiquark states

Takahashi:2002bw





Motivations

- DMC method is a mature approach in molecular physics, solid physics and nuclear physics

Reviews: Carlson:2014vla, Foulkes:2001zz; QMCPACK [https://github.com/QMCPACK/qmcpack]

- Some advantages of DMC
  - ▶ No presumed clustering
  - ▶ Milder increasing computational cost as particles numbers
  - ▶ High precision
- Applications in multiquark systems:
  - ▶ Gordillo:2020sgc

	$n^{2S+1}L_J$	J^{PC}	DMC
η_c	1^1S_0	0^{-+}	3005
J/ψ	1^3S_1	1^{--}	3101
B_c	1^1S_0	0^{-+}	6292
B_c^*	1^3S_1	1^{--}	6343
η_b	1^1S_0	0^{-+}	9424
$\Upsilon(1S)$	1^3S_1	1^{--}	9462

$cc\bar{c}\bar{c}$

J^{PC}	DMC
0^{++}	6351
1^{+-}	6441
2^{++}	6471

$$M_{T_{cc\bar{c}\bar{c}}} - 2M_{\eta_c} = 241 \text{ MeV}$$

  - ▶ Bai:2016int: $(bb\bar{b}\bar{b})$ bound states

Hjorth-Jensen:2017gss, Bai:2016int, Gordillo:2020sgc, Ma:2022vqf

Diffusion Monte Carlo

- Imaginary Schrödinger equation: $t \to i\tau$

$$-\frac{\partial\Psi(\boldsymbol{R},\tau)}{\partial\tau} = \Big[\underbrace{-\frac{\nabla^2}{2m}}_{\text{Diffusion}} + \underbrace{V(\boldsymbol{R}) - E_R}_{\text{Source or Sink}}\Big]\Psi(\boldsymbol{R},\tau), \quad \Psi(\boldsymbol{R},\tau) = \sum_i c_i\Phi_i(\boldsymbol{R})e^{-[E_i-E_R]\tau},$$

  - ▶ Diffusion equation
  - ▶ Picture: Salt in a still river
  - ▶ If we take $E_R \to E_0$, the $\Psi(\boldsymbol{R},t)$ will approach to the ground state when $t \to \infty$

- The Green's function

$$\psi(\boldsymbol{R},\tau+\Delta\tau) = \int G(\boldsymbol{R},\boldsymbol{R}',\Delta\tau)\psi(\boldsymbol{R}',\tau)d\boldsymbol{R}', \quad G = G_0G_1$$

$$G_0(\boldsymbol{R},\boldsymbol{R}',t) = (2\pi t/m)^{-3/2}e^{-\frac{m(\boldsymbol{R}'-\boldsymbol{R})^2}{2t}}, \qquad G_1(\boldsymbol{R},\boldsymbol{R}',t) = e^{-\left(\frac{V(R)+V(R')}{2}-E_R\right)t}$$

- Diffusion Monte Carlo
  - ▶ The wave function is sampled by walkers : distribution of the walkers $\Rightarrow \Psi(\boldsymbol{R},t)$
  - ▶ $\Psi_{int}(\boldsymbol{R},t)$: an state is not orthogonal to the ground state
  - ▶ Diffusion: random walk
  - ▶ Source or sink: death-birth process

Algorithm

- Walkers: in space D=3N
- Algorithm

1. Sample initial states
2. Random walk: Gaussian distribution

$$(2\pi\Delta\tau/m)^{-3/2} e^{-\frac{m(\Delta \boldsymbol{R})^2}{2\Delta\tau}},$$

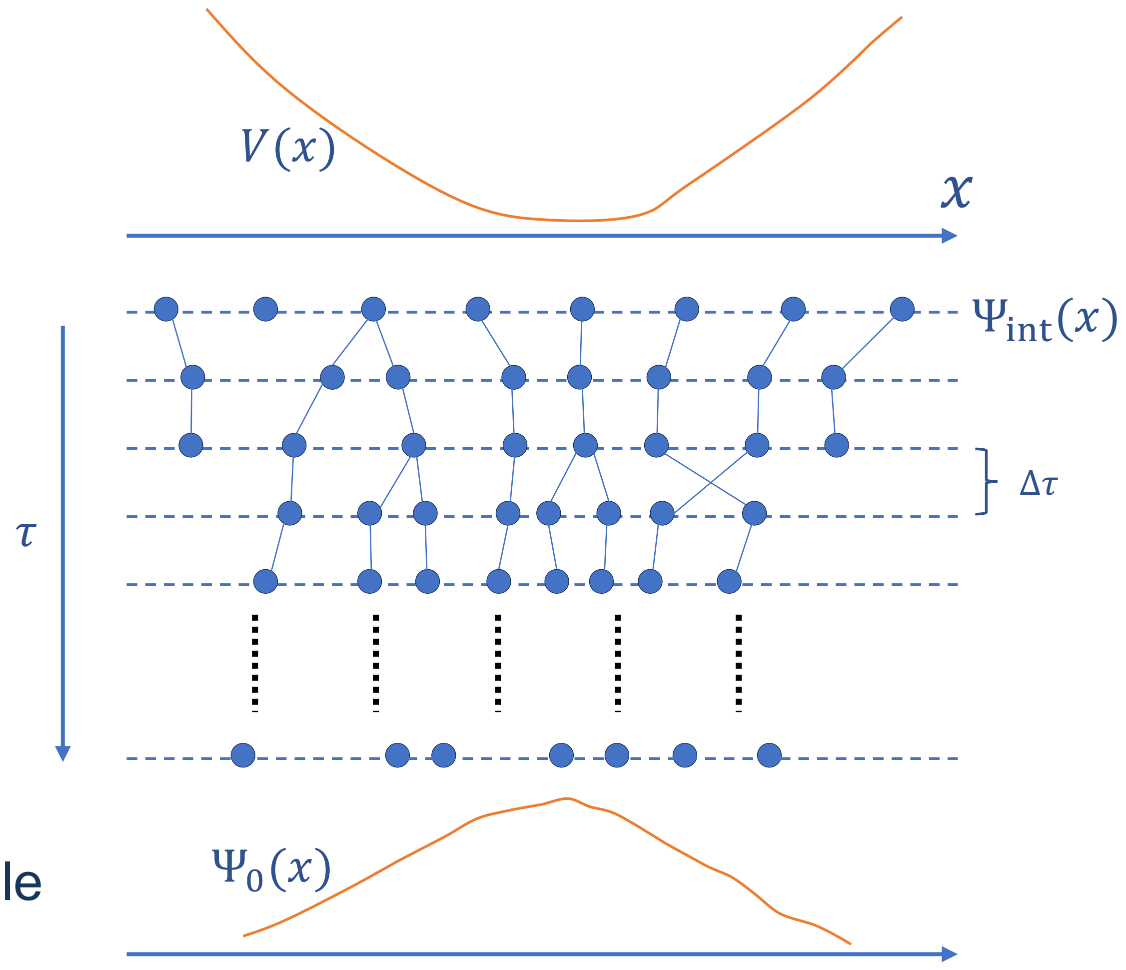
3. Death-birth: replicate the walkers n_r times

$$n_r = \text{Floor}\left[e^{-\left(\frac{V(R)+V(R')}{2}-E_R\right)\Delta\tau} + u\right]$$

   ▶ u is uniform distribution in $[0,1]$

4. Repeat 2,3…, until the equilibrium
   ▶ The distribution and total # of walkers are stable

- No numerical integration
- Manipulates in the 3D Cartesian coordinate, no partial wave expansion, no Jacob coordinate, no complex angles relations



Algorithm

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1. Sample initial states
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$$(2\pi\Delta\tau/m)^{-3/2}e^{-\frac{m(\Delta \boldsymbol{R})^2}{2\Delta\tau}},$$

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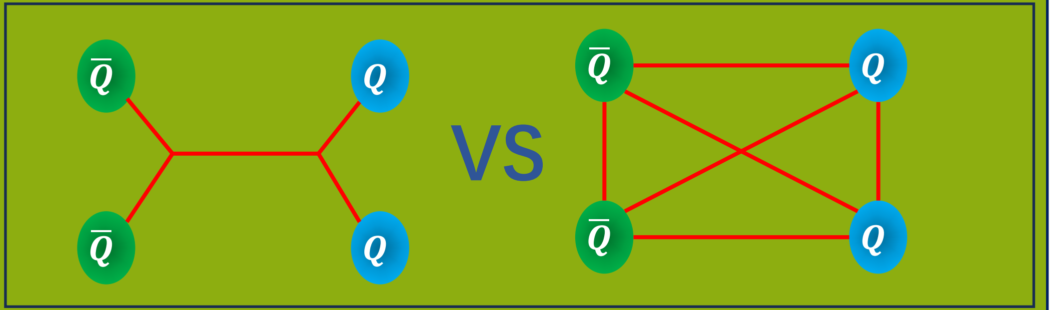
τ

In DMC method, complexity to deal with pairwise confinement interaction and flux-tube interaction are the same!!!

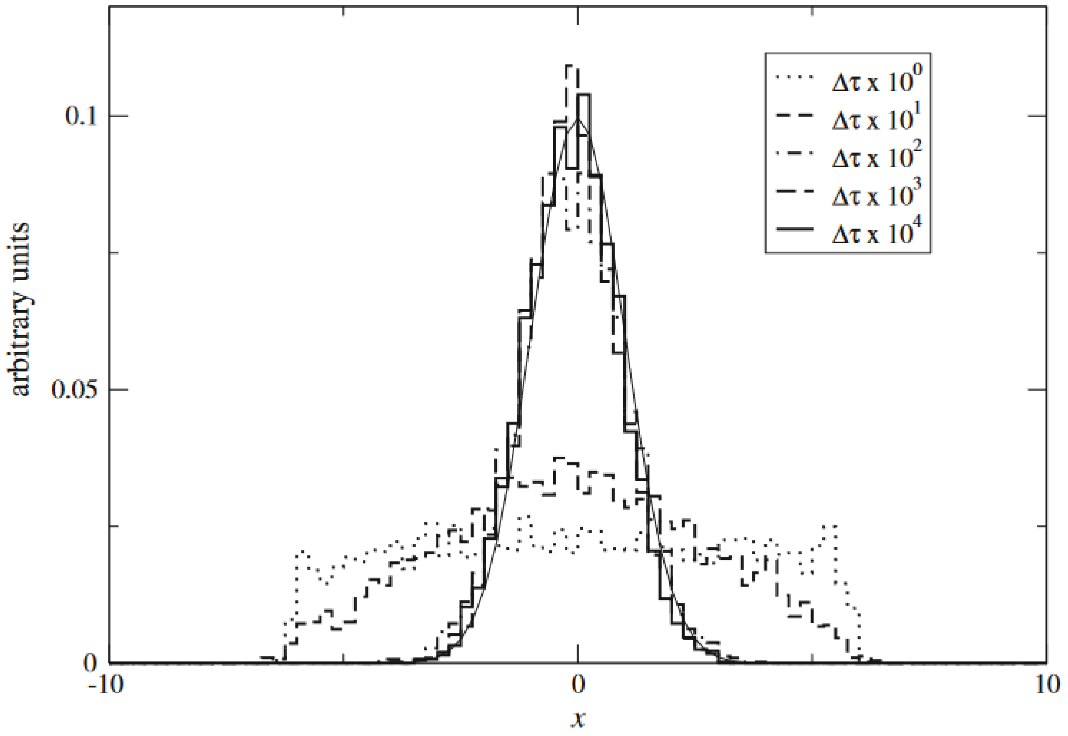


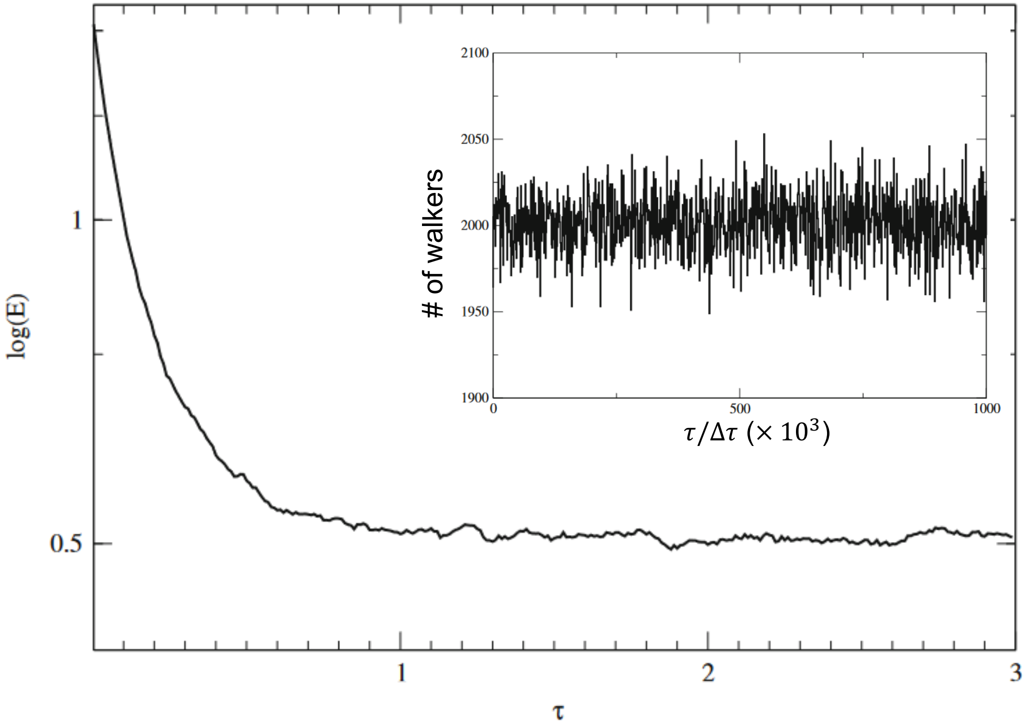
A simple example of Naïve DMC

- One-dimensional HO: $H = -\frac{1}{2}\frac{\partial^2}{\partial x^2} + \frac{1}{2}x^2$, $E_0 = 0.5$
- Initial wave functions: a constant
- Clear exponential decay of the energy towards the exact E_0
- The # of walkers depart from the central value by more than 3%

$$n_r = \mathrm{Floor}\left[e^{-\left(\frac{V(R)+V(R')}{2} - E_R\right)\Delta\tau} + u\right]$$

Walkers where the potential changes drastically, lead to large fluctuations of the population





Importance sampling

- Introduce importance function: ψ_T and sample $f(\boldsymbol{R},t)=\Psi(\boldsymbol{R},t)\psi_T(\boldsymbol{R})$
- Schrodinger equation with importance sampling

$$-\frac{\partial f(\boldsymbol{R},t)}{\partial t}=-\underbrace{\sum_{i=1}^{m}\frac{1}{2m_i}\boldsymbol{\nabla}^2_{\boldsymbol{r}_i}f(\boldsymbol{R},t)}_{\text{Random walk}}+\underbrace{\sum_{i=1}^{m}\frac{1}{2m_i}\boldsymbol{\nabla}_{\boldsymbol{r}_i}(\boldsymbol{F}_i(\boldsymbol{R})f(\boldsymbol{R},t))}_{\text{Drift}}+\underbrace{[E_L(\boldsymbol{R})-E_R]f(\boldsymbol{R},t)}_{\text{Sink or source}},$$

  - ▶ $E_L(\boldsymbol{R})=\psi_T(\boldsymbol{R})^{-1}\hat{H}\psi_T(\boldsymbol{R})$ and $\boldsymbol{F}_i(\boldsymbol{R})=2\psi_T(\boldsymbol{R})^{-1}\nabla_{r_i}\psi_T(\boldsymbol{R})=\nabla\ln|\psi_T|^2$
  - ▶ Convection–diffusion equation
  - ▶ Picture: Salt in a flowing river
- The ψ_T should approximate the Ψ_0 as closely as possible
- Green's function of drift term: $G_2(\boldsymbol{R},\boldsymbol{R}',t)=\delta(\boldsymbol{R}-\boldsymbol{R}'-\frac{\boldsymbol{F}(\boldsymbol{R}')}{2m}t)$
  - ▶ make a displacement: $\frac{\boldsymbol{F}(\boldsymbol{R}')}{2m}t$
- Function 1: guiding the walkers to regions of the wavefunction with larger amplitudes.

$$\boldsymbol{F}_i(\boldsymbol{R})=\nabla\ln|\psi_T|^2$$

- Function 2: reduces the fluctuation of the population of walkers

$$E_L(\boldsymbol{R})=\psi_T(\boldsymbol{R})^{-1}\hat{H}\psi_T(\boldsymbol{R})\to E_0$$

Hjorth-Jensen:2017gss, Bai:2016int, Gordillo:2020sgc, Ma:2022vqf

Importance sampling

- In the practical simulation, the ψ_T is unknown beforehand
- Two-body Jastow correlation factor

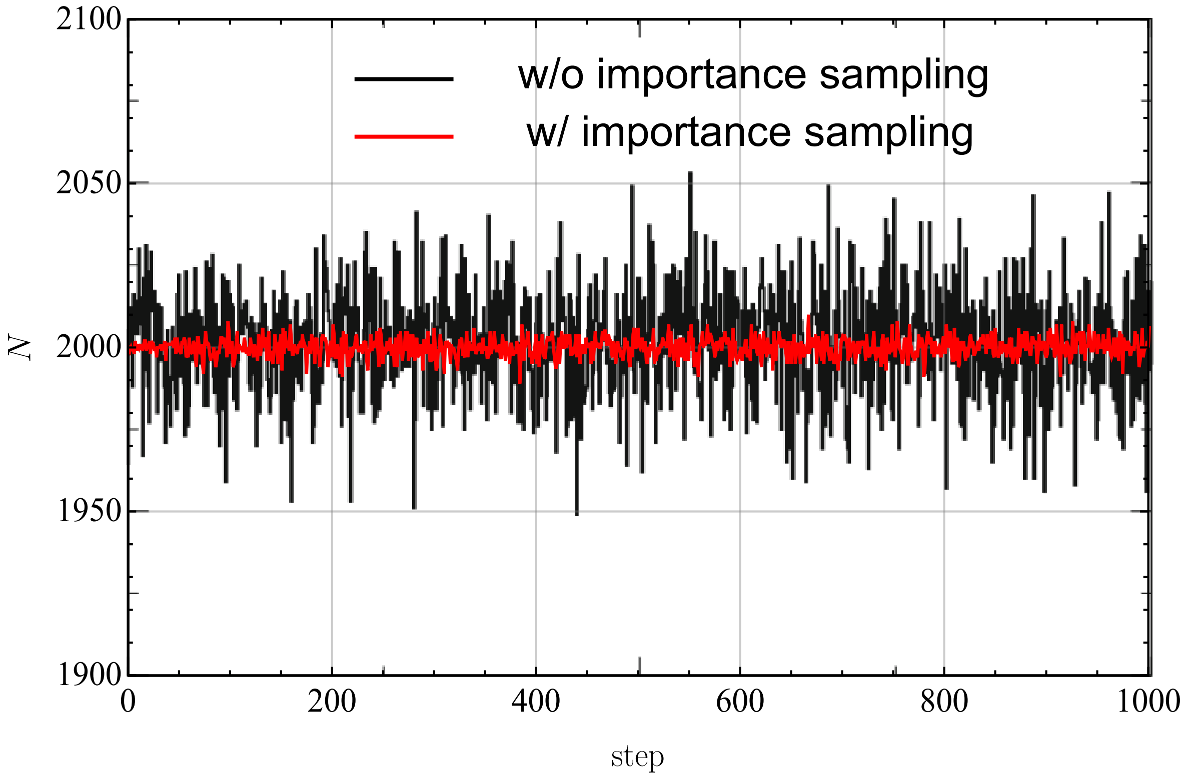
$$\psi_T(\boldsymbol{R}) = \prod_{i<j} \exp\left(\frac{a_{ij} r_{ij}}{1+\beta_{ij} r_{ij}}\right)$$

- In our calculation

$$\psi_T(\boldsymbol{R}) = \prod_{i<j} e^{-a_{ij} r_{ij}}$$

  ► a_{ij} are adjustable constants to minimize the fluctuation

- With importance sampling, the fluctuation is reduced



Coupled-channel in DMC

- Coupled channels

$$\Psi(\boldsymbol{R},t)=\sum_{\alpha}\Psi_{\alpha}(\boldsymbol{R},t)\chi_{\alpha}\,,$$

$$-\frac{\partial\Psi_{\alpha'}}{\partial t}=\sum_{\alpha}\hat{H}_{\alpha'\alpha}\Psi_{\alpha}-E_R\Psi_{\alpha'}\,.$$

- Sampling $\mathcal{F}$

$$f_{\alpha}(\boldsymbol{R},t)\equiv\psi_T(\boldsymbol{R})\Psi_{\alpha}(\boldsymbol{R},t)\,,$$

$$\mathcal{F}(\boldsymbol{R},t)\equiv\sum_{\alpha}f_{\alpha}(\boldsymbol{R},t)\,.$$

- Assuming $\mathcal{F}$ is positive such that can be sampled by distribution of walkers

Gordillo:2020sgc

Baryons

- We choose the AL1 and its revise versions
- Two different confinement scenarios
- In variational method: It is hard to calculate the matrix elements of V_{conf}^{Y}

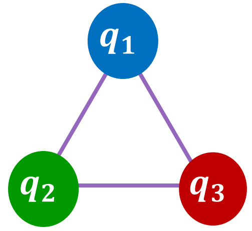
$$\int d\vec{\rho} d\vec{\lambda} \psi_i^*(\vec{\rho},\vec{\lambda}) L_{\min}(\rho,\lambda,\cos(\hat{\rho},\hat{\lambda}))\psi_j(\vec{\rho},\vec{\lambda})$$

$$L_{min} = [\tfrac{1}{2}(a^2+b^2+c^2)+\tfrac{\sqrt{3}}{2}\sqrt{(a+b+c)(-a+b+c)(a-b+c)(a+b-c)}]^{1/2}$$

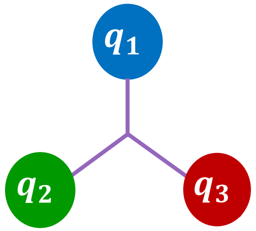
  - ▶ Numerical integration
  - ▶ For the tetraquark states: no analytical results, Smiths algorithm
- In DMC method, the flux tube interaction: No extra computational cost
  - ▶ Walkers in 3N Cartesian coordinate
- Using Smiths algorithm to prepare for the tetraquark calculation in the future

D. Smith, Algorithmica 7, 137 (1992)

- Coupling constants
  - ▶ σ_Δ from AL1 model
  - ▶ Flux tube-I: $\sigma_Y = \sigma_{\bar{q}q} = 2\sigma_\Delta$, Flux tube-II: fix σ_Y from $\Omega(sss)$ mass, $\sigma_Y = 0.9204\sigma_{\bar{q}q}$



$V_{\rm conf}^{\Delta} = \sigma_\Delta \sum_{i<j} r_{ij}$



$V_{\rm conf}^{Y} = \sigma_Y L_{min}$

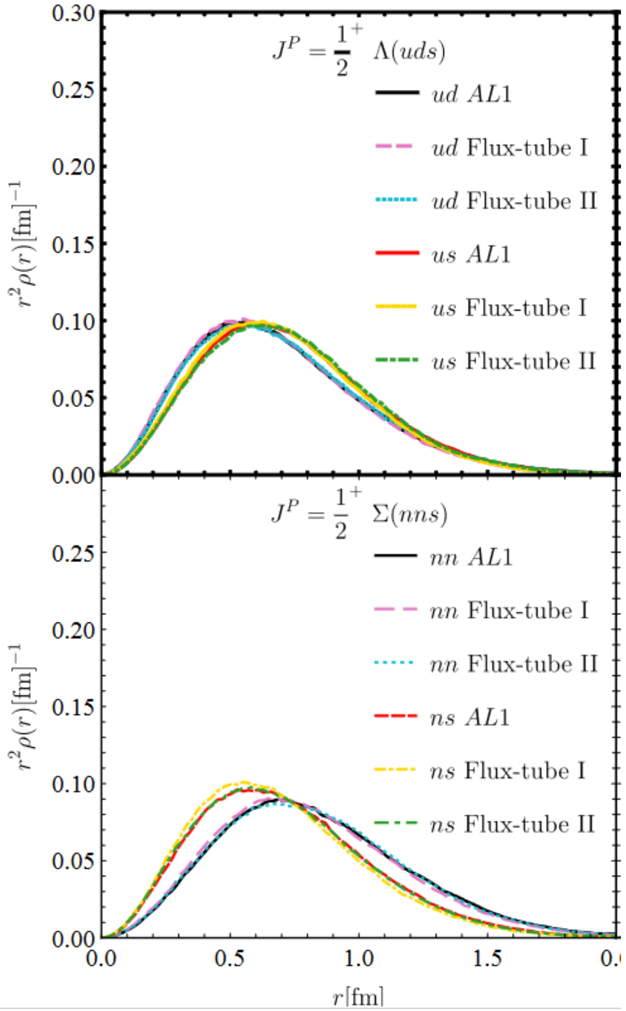
Takahashi:2002bw Lattice QCD: $\sigma_Y = 0.9355\sigma_{\bar{q}q}$

Results of baryon

- A lesson from nucleon calculation: include the basis completely
  - ▶ $|N\rangle_{fac} = \chi_{SIC}(1,2,3)^A \times \psi^S(r_1, r_2, r_3)$: not general enough
  - ▶ Other basis

$$|\psi\rangle = \chi_{SIC}(1,2;3)^A \times \psi^S(r_1 r_2; r_3) + Antisymetrization$$

	AL1			Flux-tube-I	Flux-tube-II	Exp.
	DMC	GEM	Faddeev	DMC	DMC	
$\|N\rangle_{fac}$	968	966	-	-	-	939
Complete	930	930	933	1059	975	



- The flux-tube potential is doable
- Flux-tube-II is more reliable
- For baryons it is hard to distinguish two confinement mechanisms

$$0.5 \leq \frac{L_{min}}{L_\Delta} \leq 0.58$$

- ▶ More complicate spatial configurations for tetraquark state

Could be used to distinguish different confinement scenarios

DMC in quark models

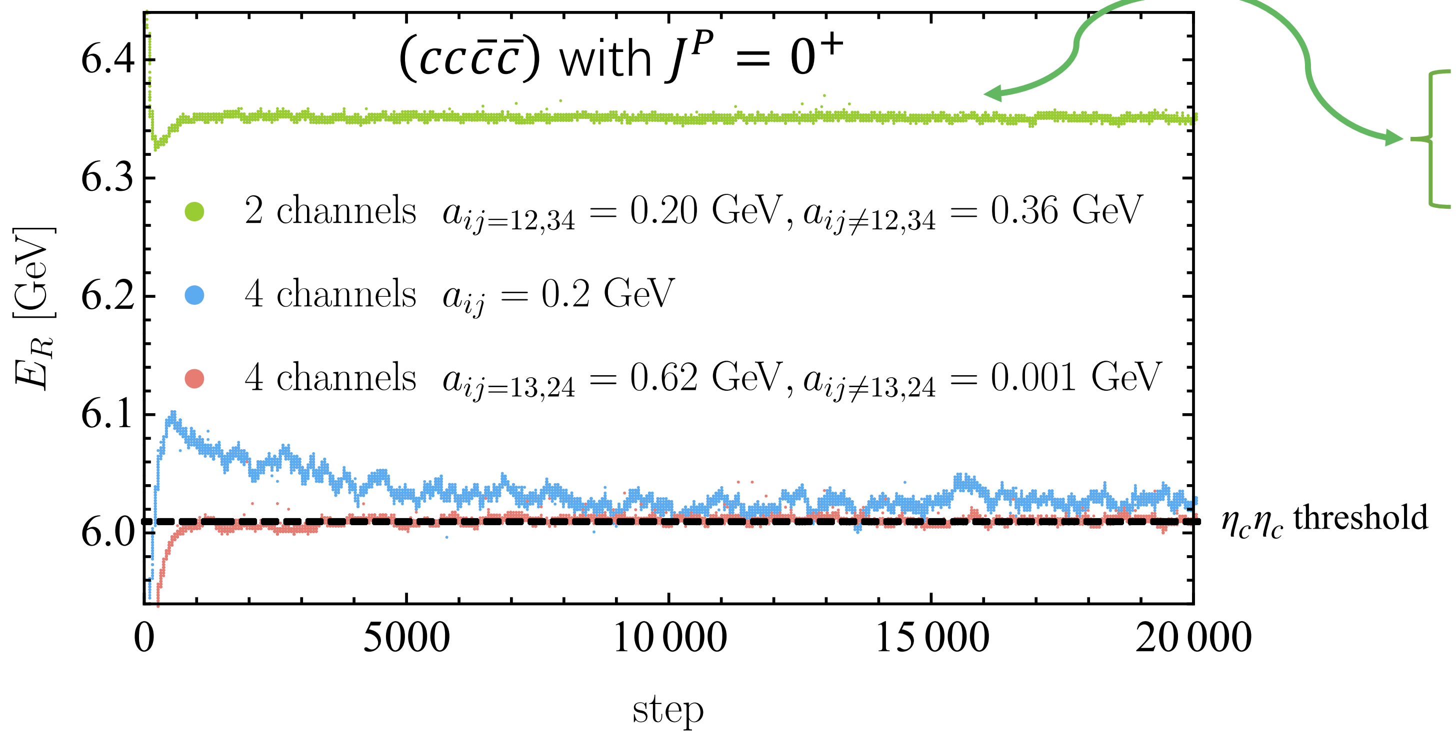
- Cannot get the di-meson thresholds (real ground state) for the systems w/o bound states

Gordillo:2020sgc

- Our advancement: including the extra two channels
  - ▶ Obtain the di-meson thresholds independent of the importance functions

Ma:2022vqf

Gordillo:2020sgc



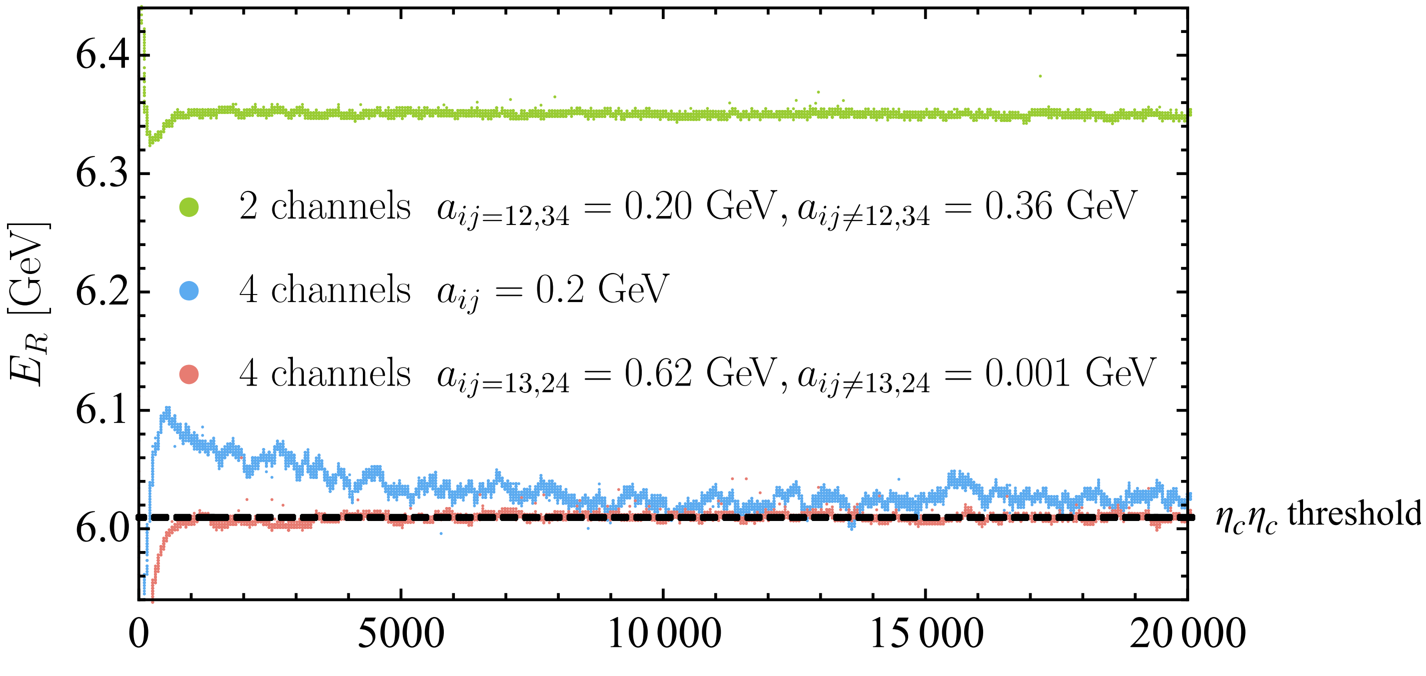
$$|T1\rangle = \left[(12)^{0_s}_{\bar{3}_c}(34)^{0_s}_{3_c}\right]^{0_s}_{1_c}\psi_1^{SS}(12;34),$$
$$|T2\rangle = \left[(12)^{1_s}_{6_c}(34)^{1_s}_{\bar{6}_c}\right]^{0_s}_{1_c}\psi_2^{SS}(12;34)$$
$$|T3\rangle = \left[(12)^{1_s}_{\bar{3}_c}(34)^{1_s}_{3_c}\right]^{0_s}_{1_c}\psi_3^{AA}(12;34),$$
$$|T4\rangle = \left[(12)^{0_s}_{6_c}(34)^{0_s}_{\bar{6}_c}\right]^{0_s}_{1_c}\psi_4^{AA}(12;34)$$

Ours

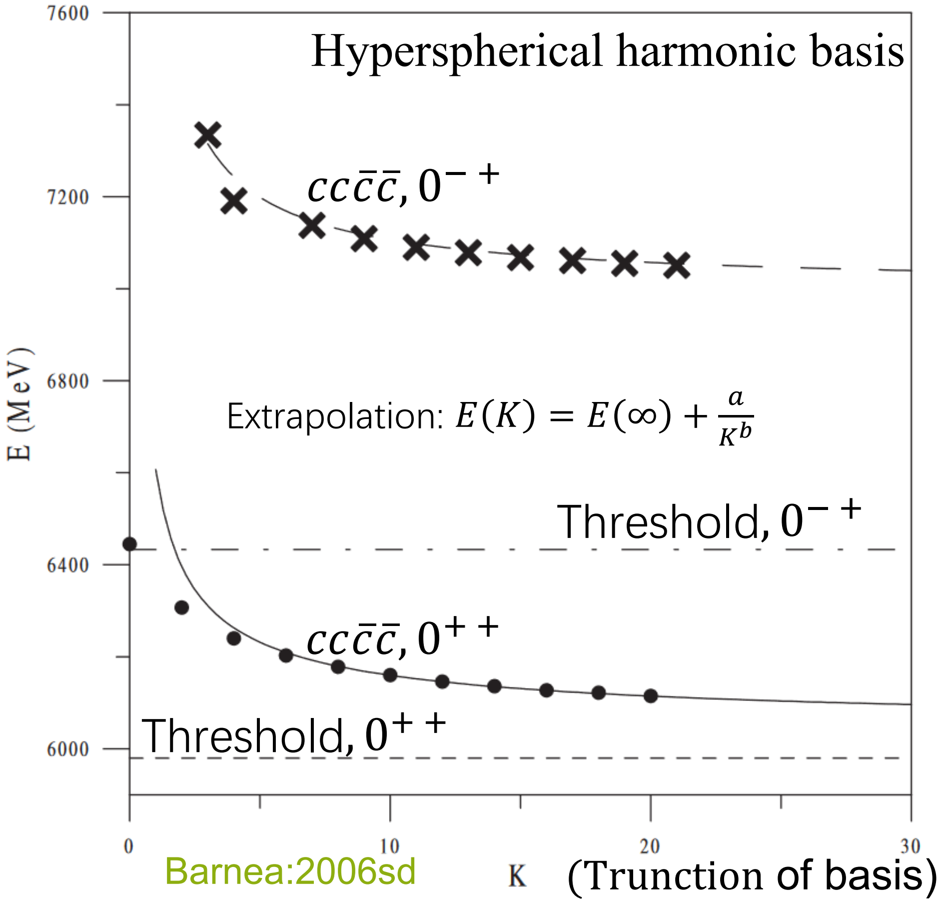
$$\psi_T(\boldsymbol{R}) = \prod_{i<j} e^{-a_{ij}r_{ij}} .$$

DMC in quark models

- Get a di-meson type ground state without presumed such kind of correlation
  - ▶ The importance wave function with even two-body correlations give the di-meson thresh. $a_{12} = a_{13} = a_{23} = a_{14} = a_{23} = a_{34}$
- In variational method, it is hard to get the di-meson without the di-meson type in basis
- No need presumed clustering behaviors!!!



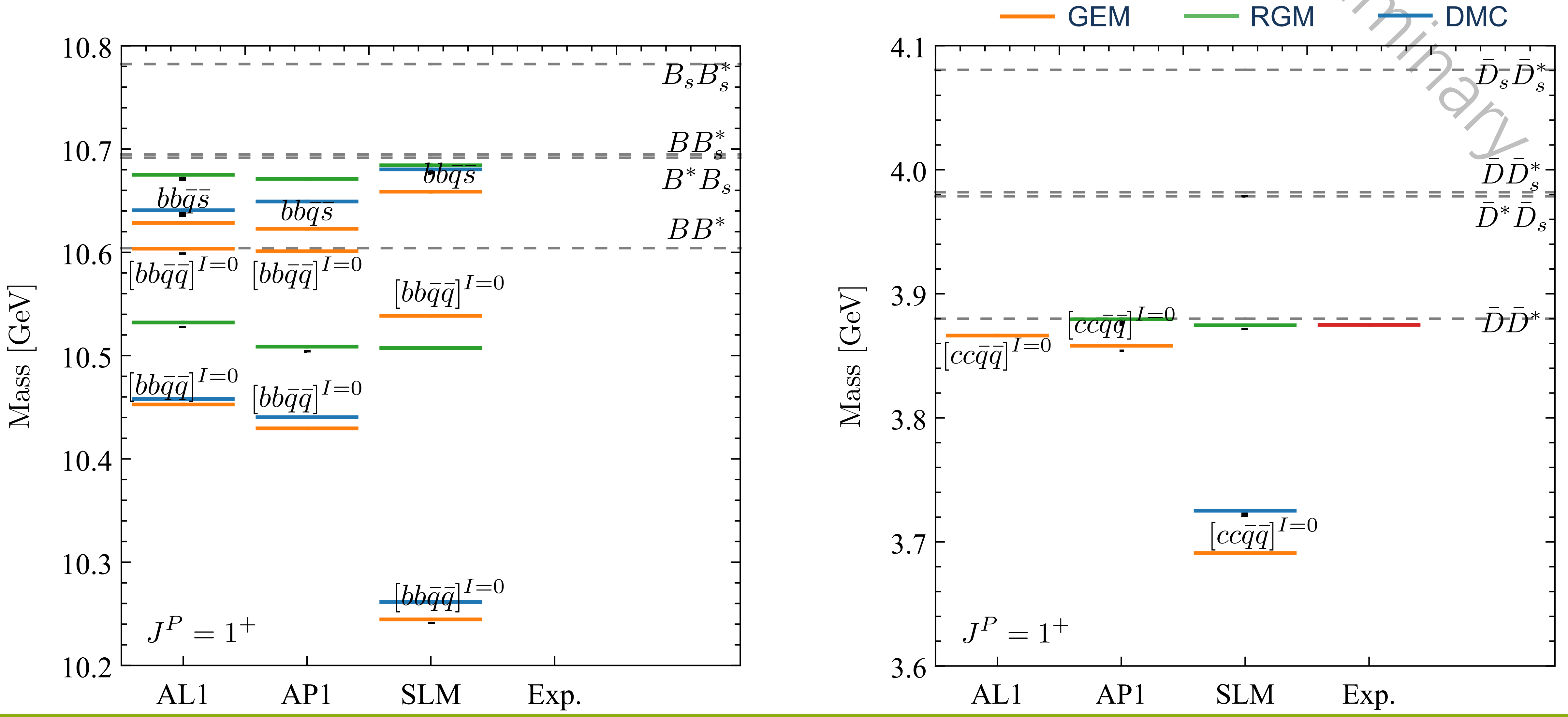
$$\psi_T(\boldsymbol{R}) = \prod_{i<j} e^{-a_{ij}r_{ij}} .$$



Barnea:2006sd

Results from DMC

- The DMC with the present coupled-channel strategy give the higher energy than GEM
- The DMC performs better than RGM



Systemic uncertainties

- Time-step uncertainty
- Walker number control uncertainty
- Choice of importance wave functions
- Fermion sign problem (Main problem)
  - ▶ The density of the walker is always positive
  - ▶ However, the wave functions can be negative
  - ▶ The present coupled channel strategy
  - ▶ Better choice: fixed-node method, fixed-phase method…
- Other possible improvement
  - ▶ The wave function of the discrete quantum numbers can be sampled
    Auxiliary field diffusion Monte Carlo
  - ▶ Optimize the initial function and importance function

Summary and outlook

- Investigate the tetraquark bound states with (AL1,AP1,SLM)⊗(GEM,RGM,DMC)
  - ► $(QQ\bar{Q}\bar{Q})$, $(QQ\bar{Q}\bar{q})$, $(QQ\bar{q}\bar{q})$, $(Qs\bar{q}\bar{q})$, $(Q\bar{s}q\bar{q})$
- Recommended tetraquark states below di-meson thresholds (consistent predictions of 3 models)

$J^P=1^+$	$[cc\bar{q}\bar{q}]^{I=0}$	$[bb\bar{q}\bar{q}]^{I=0}$	$[bc\bar{q}\bar{q}]^{I=0}$	$bb\bar{q}\bar{s}$	$[bs\bar{q}\bar{q}]^{I=0}$
$J^P=0^+$	$[cb\bar{q}\bar{q}]^{I=0}$	$[cs\bar{q}\bar{q}]^{I=0}$	$[bs\bar{q}\bar{q}]^{I=0}$		
$J^P=2^+$	$[cb\bar{q}\bar{q}]^{I=0}$				

- Unfortunately, disagreements in three methods
- GEM performs the best for bound states calculations
- RGM: not general enough to give the ground bound state
  - ► For quark models born with RGM, it is inconsistent to include diquark-antidiquark correlations
  - ► Promising to deal with resonance states
- DMC: improved to give the di-meson threshold
  - ► Can be further improved: Auxiliary field diffusion Monte Carlo, fixed-node method
  - ► Flux-tube confinement potentials for tetraquark states
  - ► Resonance state by putting the few-body system into finite box or a well

Thanks for your attention!

Backup

Resonances within DMC method

- Put them into finite box or a well Wiese:1988qy, Gandolfi:2016bth
- Similar to the real scaling method
- More methods to calculate resonance: see the papers about tetra-neutron resonance

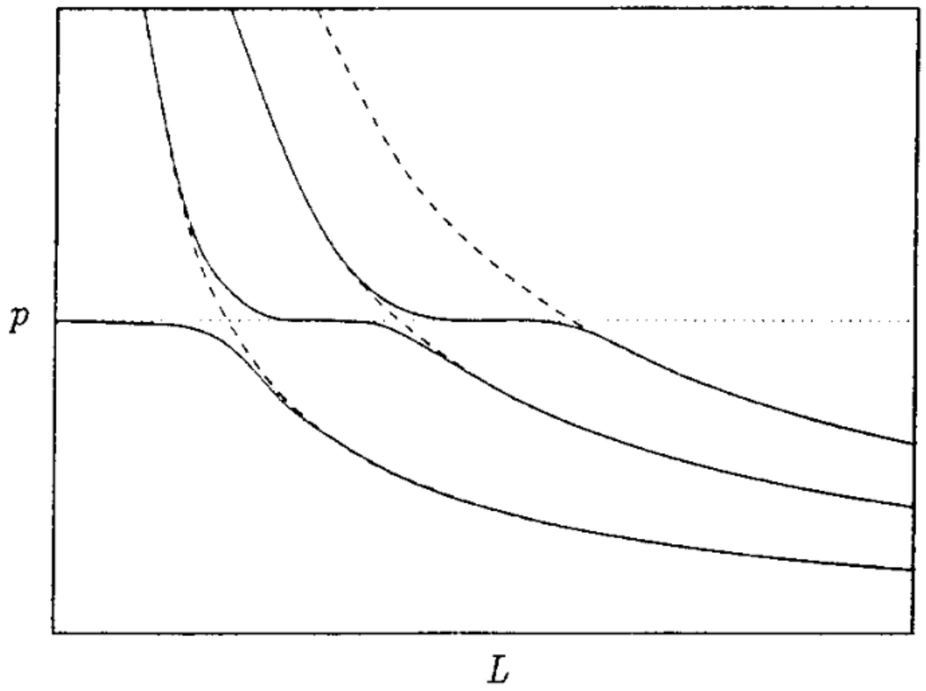
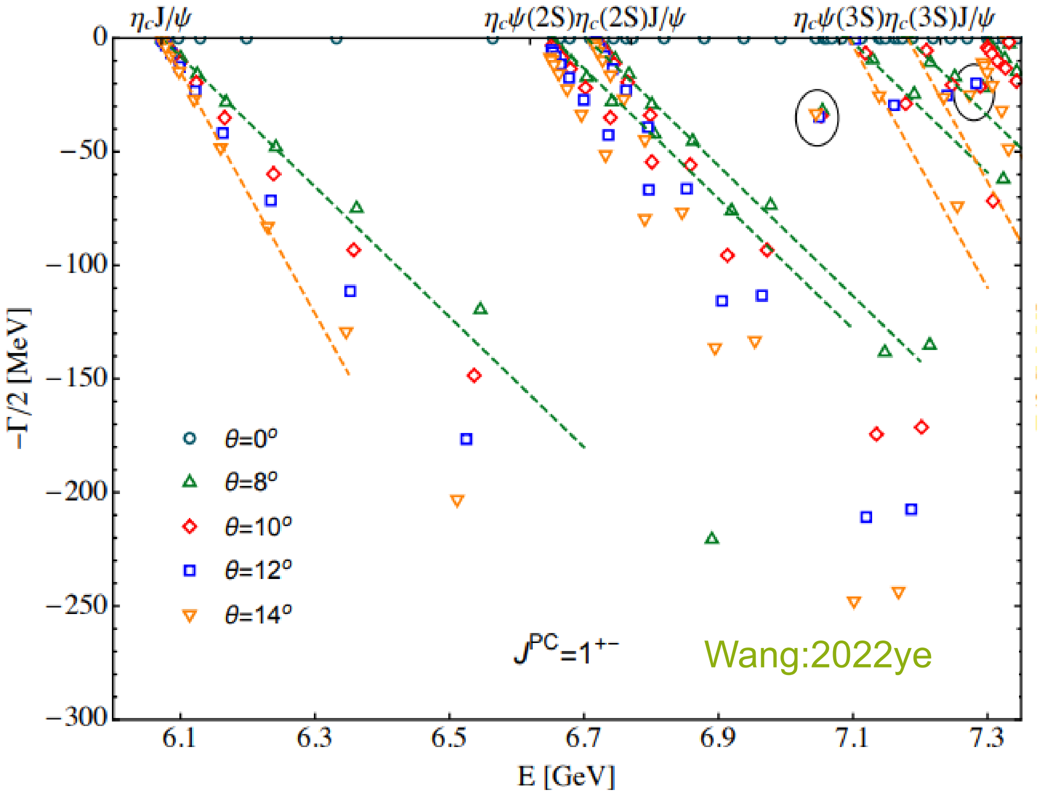


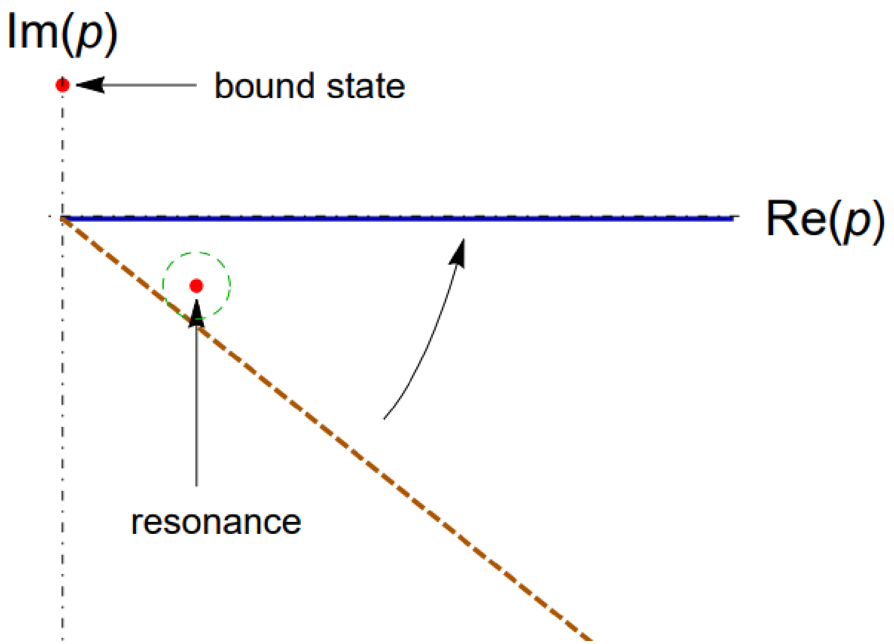
Figure 2: The finite volume spectrum of the free and the interacting model. Wiese:1988qy

Methods to obtain resonance and virtual states

- Complex scaling methods with GEM
  - ▶ It is hard to detect the higher states
  - ▶ The unclear relation with Riemann surface
  - ▶ The tetraquark resonance: two-body scattering problems (confinement)
- RGM + Complex Scaling in coupled-channel two-body problem



Solving Freedholm determinant⇒ Eigenvalue problem



Comparison

TABLE VI. Mass and binding energy (in MeV/c^2) and probabilities of each channel (in %) for the $J^P = 1^+$ T_{bb} states predicted in this work.

Mass	E_B	$\mathcal{P}_{B^0 B^{*+}}$	$\mathcal{P}_{B^+ B^{*0}}$	$\mathcal{P}_{B^{*+} B^{*0}}$	$\mathcal{P}_{I=0}$	$\mathcal{P}_{I=1}$
10582.2	21.9	47.8	50.0	2.2	99.99	0.01
10593.5	10.5	51.0	48.6	0.4	0.02	99.98

Our results: there is no isospin vector states

TABLE VI. Mass and binding energy (in MeV/c^2) and probabilities of each channel (in %) for the $J^P = 1^+$ T_{bb} states predicted in this work.

Mass	E_B	$\mathcal{P}_{B^0 B^{*+}}$	$\mathcal{P}_{B^+ B^{*0}}$	$\mathcal{P}_{B^{*+} B^{*0}}$	$\mathcal{P}_{I=0}$	$\mathcal{P}_{I=1}$
10582.2	21.9	47.8	50.0	2.2	99.99	0.01
10593.5	10.5	51.0	48.6	0.4	0.02	99.98

TABLE VII. Properties of the T_{bb} candidates as $B^{(*)}B^{(*)}$ molecules in the $J^P = 0^+$ and 2^+ sectors obtained in this work. Masses, widths, binding energies and partial widths are shown in MeV/c^2.

J^P	I	Mass	Width	E_B	$\mathcal{P}_{BB}$	$\mathcal{P}_{B^*B^*}$	Γ_{BB}	$\Gamma_{B^*B^*}$
0^+	0	10553.0	0	6.0	92%	8%	0	0
		10640.7	2.8	8.7	76%	24%	2.8	0
	1	10545.9	0	13.1	93%	7%	0	0
		10672.6	72.0	−23.2	39%	61%	30.7	41.3
2^+	1	10642.3	0	7.1	-	100%	-	0

The S-wave BB states can not be $J^P(I) = 0^+(0)$

Fermion sign problem in DMC

- The density of the walker is always positive
- In principle, the mathematical ground state of few-body system has no node
- Considering the identical particles, the Antisymmetrization of the fermions introduce the nodes
- For boson systems, the excited state wave functions have nodes
- How to get $\psi(R)$ with negative part?
- Naive strategy:
  - $\psi(R) = \psi^+(R) - \psi^-(R)$, $\psi^+(R) > 0$ and $\psi^-(R) > 0$
  - Give each walker a label: (+) or (-) to sample $\psi^+(R)$ and $\psi^-(R)$ respectively
  - $\psi^+(R)$ and $\psi^-(R)$ will approach to the same mathematical ground state $\psi_0(r)$
  - Significant cancellation!!! Large noise!!! Fermin sign problem
- Fix node: kill the walker across the nodal surface

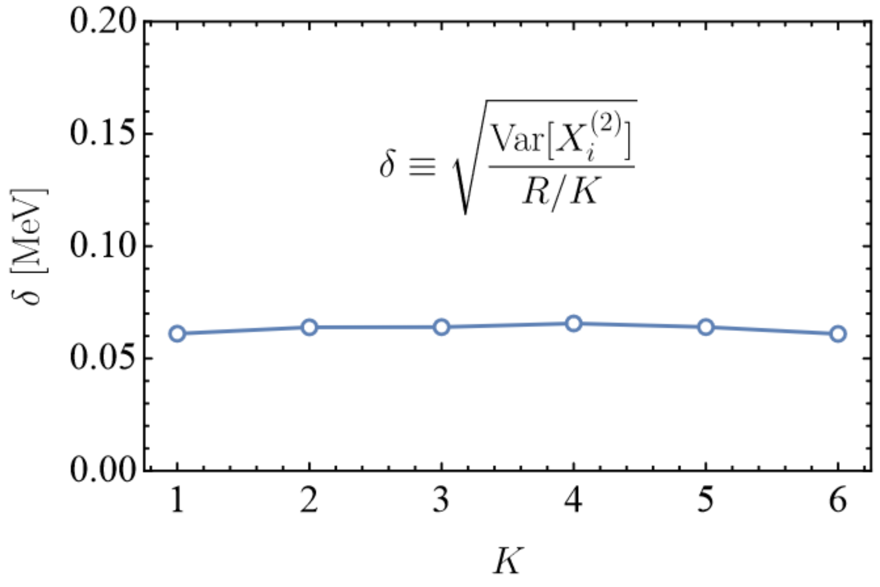
Statistical uncertainties of DMC

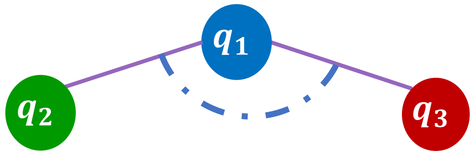
- Jackknife resampling method

$$\sigma[\bar{X}] = \sqrt{\frac{1}{R(R-1)}\sum_i^R (X_i^{(1)} - \bar{X})^2}$$

$$= \sqrt{\frac{R-1}{R}\sum_i^R (\bar{X}_{(i)\mathrm{jack}} - \bar{X}_{\mathrm{jack}})^2}\,.$$

- Statistical uncertainties: less than 1 MeV





q_1
q_2
q_3

Proton results

$$|N\rangle_{\rm frac} = \chi^S_{sf}(123)\psi^S(123),$$

$$|A1\rangle = \chi^S_s(12;3)\chi^S_f(12;3)\psi_1(1;2;3),$$
$$|A2\rangle = \chi^S_s(12;3)\chi^A_f(12;3)\psi_2(1;2;3),$$
$$|A3\rangle = \chi^A_s(12;3)\chi^A_f(12;3)\psi_3(1;2;3),$$
$$|A4\rangle = \chi^A_s(12;3)\chi^S_f(12;3)\psi_4(1;2;3).$$

$$|B1\rangle = \chi^S_s(12;3)\chi^S_f(12;3)\psi^S_1(12;3),$$
$$|B2\rangle = \chi^S_s(12;3)\chi^A_f(12;3)\psi^A_2(12;3),$$
$$|B3\rangle = \chi^A_s(12;3)\chi^A_f(12;3)\psi^S_3(12;3),$$
$$|B4\rangle = \chi^A_s(12;3)\chi^S_f(12;3)\psi^A_4(12;3),$$

$$|Ci\rangle = |Bi\rangle + \text{even perm. (1,2,3)}$$

	AL1			FT I	FT II	Exp
	DMC	VAR	Faddeev			
$\lvert N(123)\rangle_{\rm fac}$	968	966		1059	975	
$\lvert C1\rangle$	/	944		/	/	
$\lvert C3\rangle$	/	931		/	/	
$\lvert C1\rangle, \lvert C3\rangle$	/	930	933	/	/	939
$\lvert C1\rangle, \lvert C2\rangle, \lvert C3\rangle, \lvert C4\rangle$	/	930		/	/	
$\lvert B1\rangle, \lvert B2\rangle, \lvert B3\rangle, \lvert B4\rangle$	/	930		/	/	
$\lvert A1\rangle, \lvert A2\rangle, \lvert A3\rangle, \lvert A4\rangle$	930	930		1019	936	