*The 7th Symposium on "Symmetries and the emergence of Structure in QCD"*

# Baryons and Tetraquark States with Diffusion Monte Carlo Method

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

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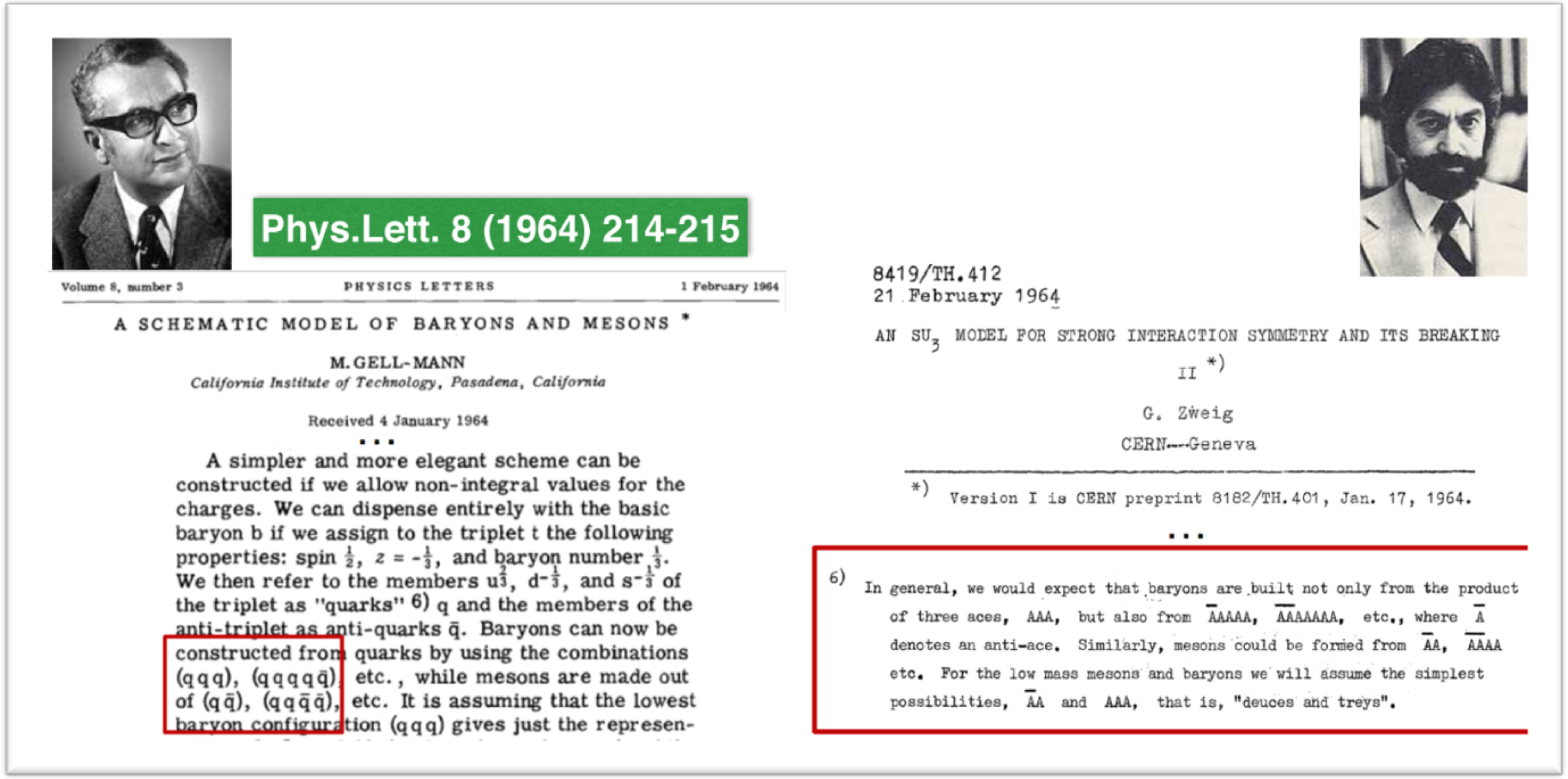
***July 21, 2023, Rizhao***

# Contents

# Multiquark state



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 $(qqq)$, $(qqqq\bar{q})$, etc., while mesons are made out of $(q\bar{q})$, $(qq\bar{q}\bar{q})$, etc. It is assuming that the lowest baryon configuration $(qqq)$ 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

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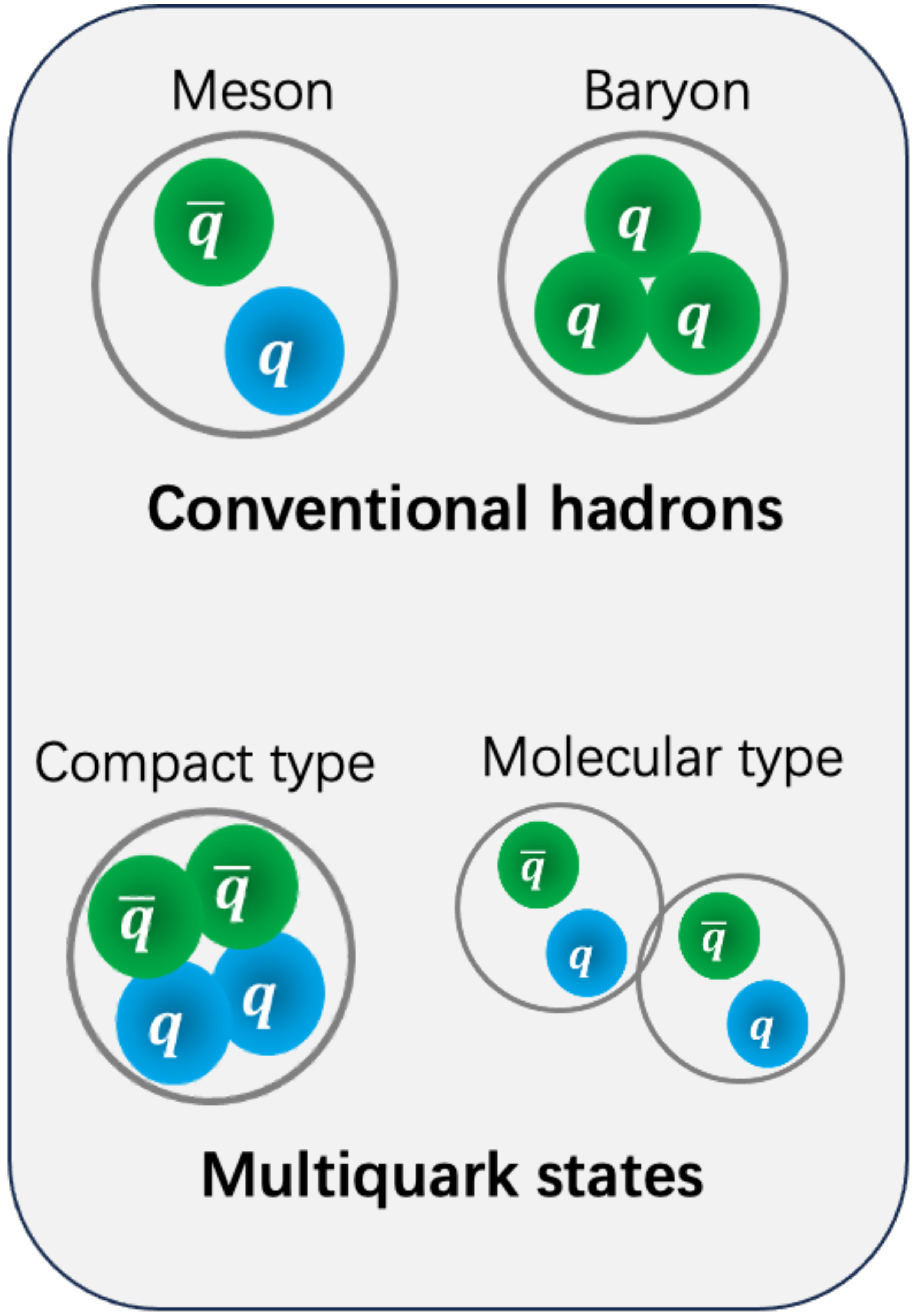
*) Version I is CERN preprint 8182/TH.401, Jan. 17, 1964.

...

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



- Multiquark states were predicted at the birth of quark model
- Quark model——a useful theoretical tool

◆ Cornell model:

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

Eichten:1974af,Eichten:1978tg,Eichten:1979ms

# Quark potential model

- Semay-Silvestre-Brac Models

Semay:1994ht,Silvestre-Brac:1996myf

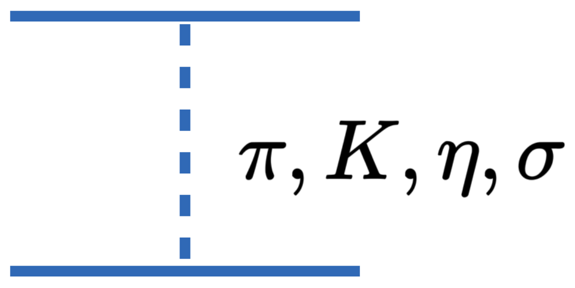
$$V_{ij}(r) = \left[-\frac{\kappa}{r} + \lambda r^p - \Lambda + \frac{2\pi}{3m_i m_j}\kappa' \frac{1}{\pi^{3/2} r_0^3} e^{(-r^2/r_0^2)} \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j\right] \lambda_i \cdot \lambda_j$$

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

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

Vijande:2004he, Segovia:2011dg

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



- Flux-tube confinement - three-body and four-body force

Takahashi:2002bw

# Motivation

## Variational method

- Computational cost increases exponentially with # of particles
- Three-body and four-body force
- Presumed clustering

## Diffusion Monte Carlo (DMC) Method

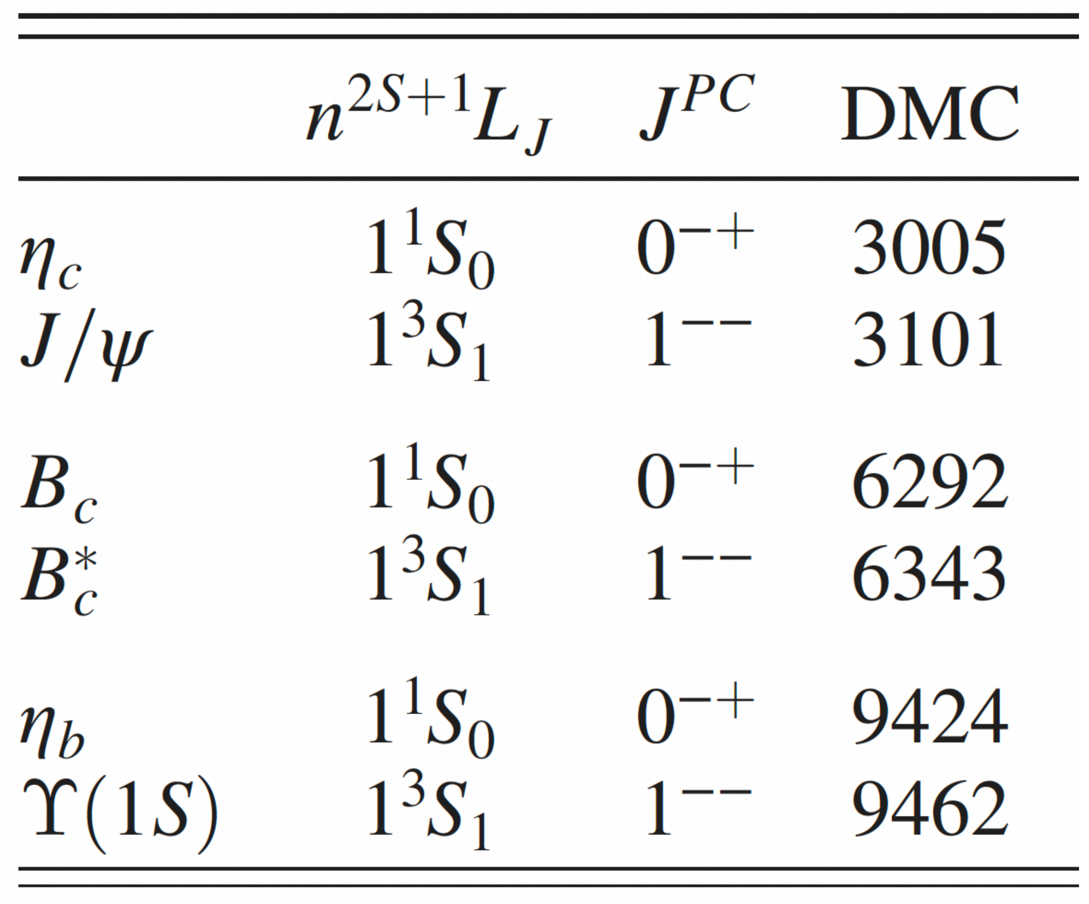
Reviews: Carlson:2014vla, Foulkes:2001zz

— —a mature approach in molecular physics, solid physics and nuclear physics

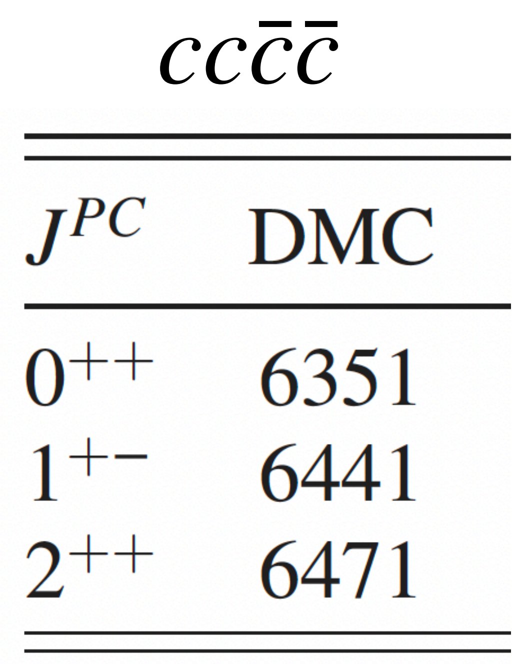
- Moderate the increasing computational cost as the particles number
- Easier to deal with the few-body force
- No presumed clustering

## DMC applications in multiquark systems

Gordillo:2020sgc



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



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

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

$$M_{T_{cc\bar{c}\bar{c}}} - 2M_{\eta_c} = 341 \text{ MeV}$$

Bai:2016int

$bb\bar{b}\bar{b}$, $0^{++}$ bound state

# Diffusion Monte Carlo (DMC) Method

# Diffusion Monte Carlo

- A numerical way for solving Schrödinger equation
- Imaginary time Schrödinger equation ($\tau = it$)

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

  - Diffusion equation: Salt in still water
  - If we take $E_R = E_0, \quad \lim_{\tau \to \infty} \Psi(\boldsymbol{R},\tau) = c_0 \Phi_0(\boldsymbol{R})$

- Solution in the form of path integral

$$\begin{aligned}\Psi(\boldsymbol{R},\tau+\Delta\tau) &= \int G\left(\boldsymbol{R},\boldsymbol{R}',\Delta\tau\right)\Psi\left(\boldsymbol{R}',\tau\right)d\boldsymbol{R}' \\ &= \int G_1\left(\boldsymbol{R},\boldsymbol{R}',\Delta\tau\right)G_2\left(\boldsymbol{R}',\boldsymbol{R}'',\Delta\tau\right)\Psi\left(\boldsymbol{R}'',\tau\right)d\boldsymbol{R}'d\boldsymbol{R}''\end{aligned}$$

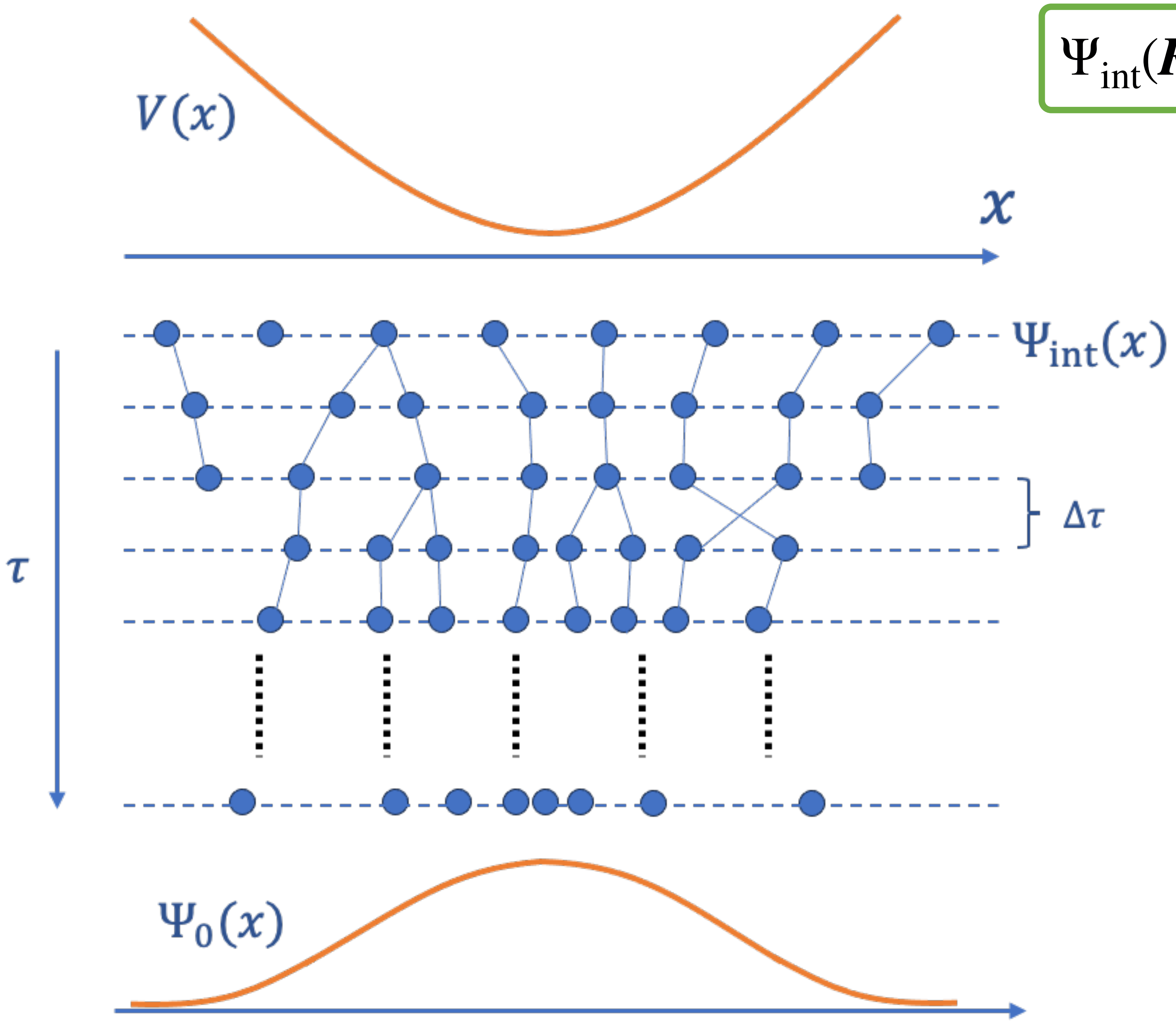
- The Green's function

$$G_1\big(\boldsymbol{R},\boldsymbol{R}',t\big) = (2\pi t/m)^{-3/2} e^{-\frac{m\left(\boldsymbol{R}'-\boldsymbol{R}\right)^2}{2t}}, \; G_2\big(\boldsymbol{R},\boldsymbol{R}',t\big) = e^{-\left(\frac{V(\boldsymbol{R})+V\left(\boldsymbol{R}'\right)}{2} - E_R\right)t}$$

  - Can be implemented with the diffusion Monte Carlo algorithm

# Algorithm

- The wave function is sampled by walkers: $\Psi(\boldsymbol{R}) \Rightarrow$ distribution of walkers
- Walkers: in space D=3N



$\Psi_{\text{int}}(\boldsymbol{R})$: a state not orthogonal to the ground state

Follow the Gaussian distribution:

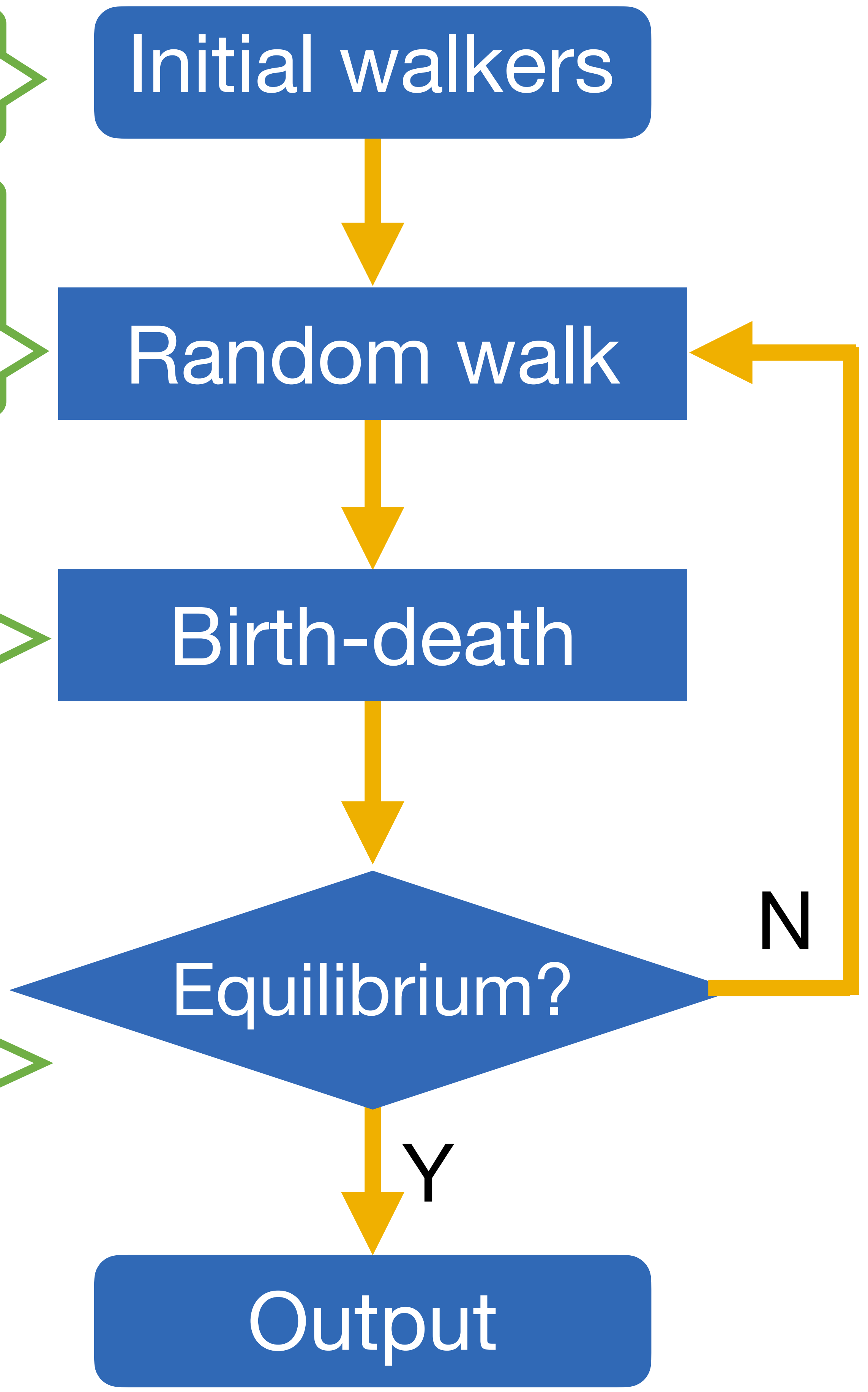
$$(2\pi\Delta\tau/m)^{-3/2}e^{-\frac{m(\Delta R)^2}{2\Delta\tau}}$$

Replicate the walker $n_r$ times:

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

◆ $u$ is a random number uniformly distributed in $[0,1]$

$E_R$ and total # of walkers become stable?



Initial walkers

Random walk

Birth-death

Equilibrium?

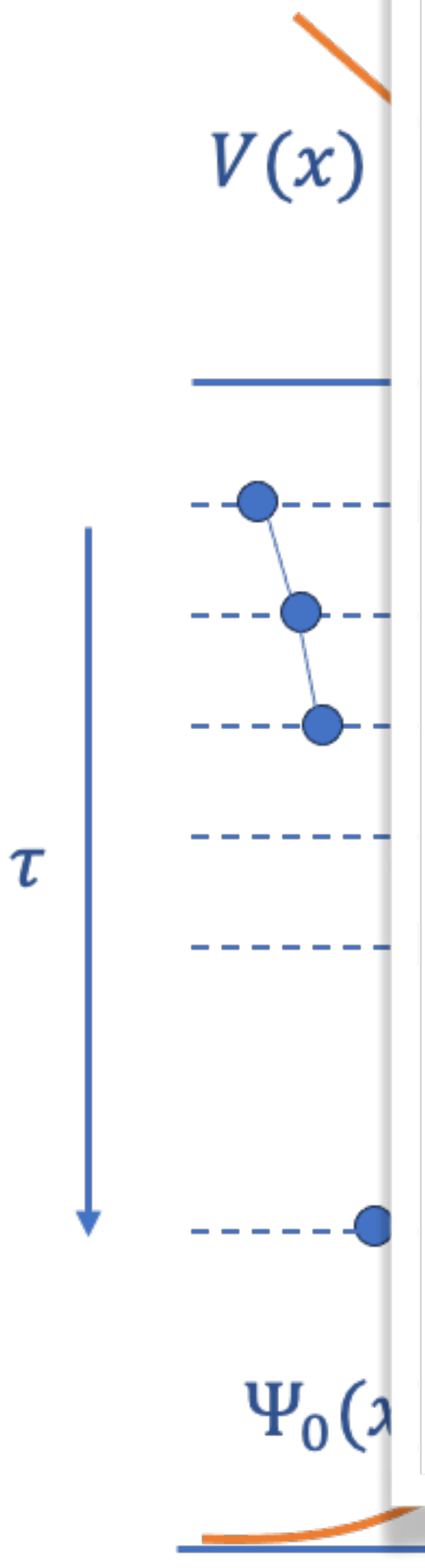
N

Y

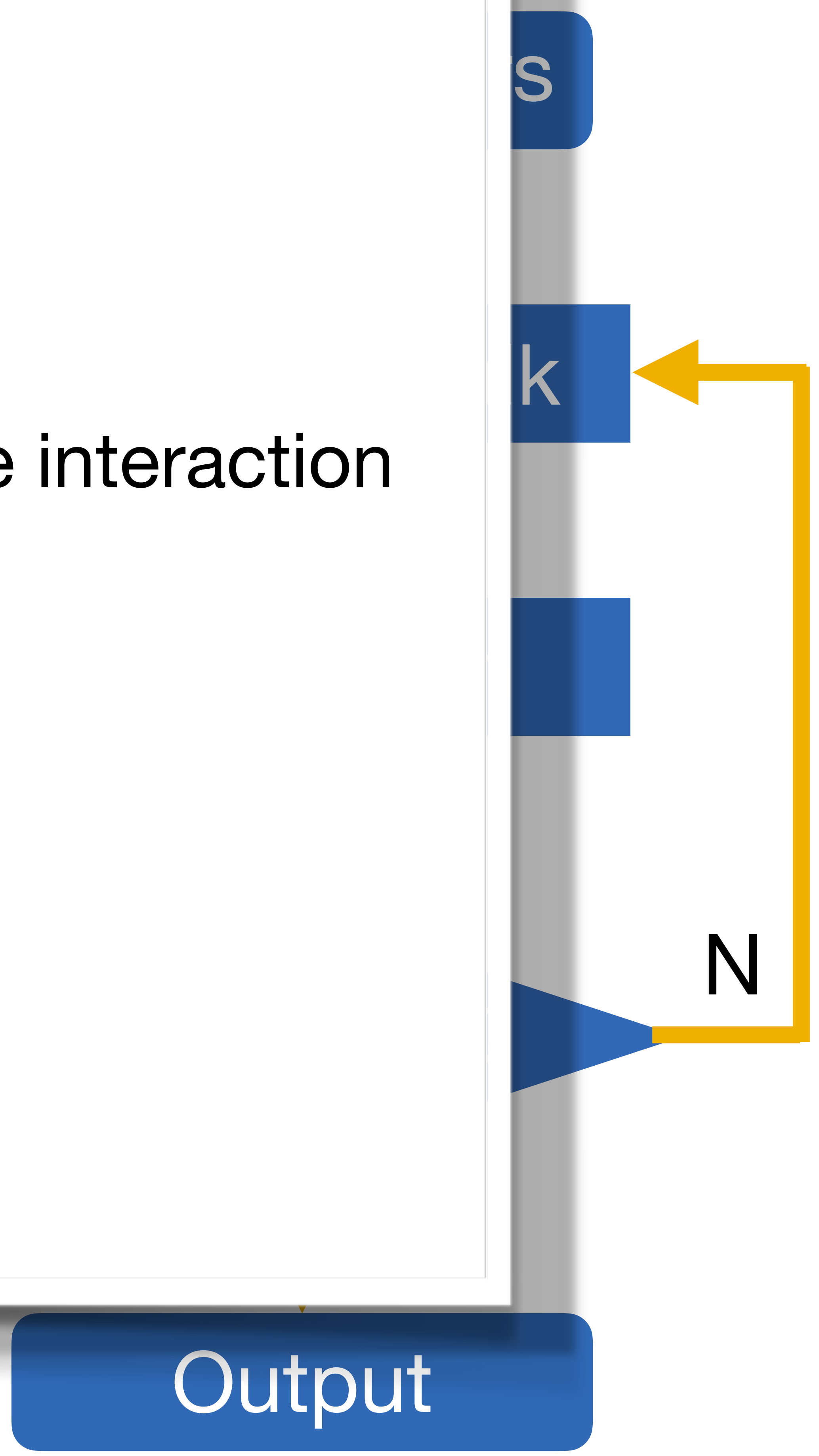
Output

# Algorithm

- The wave function is sampled by walkers: $\Psi(\boldsymbol{R}) \Rightarrow$ distribution of walkers
- Walkers: in space D=3N



- No numerical integration
- No Jacobi coordinate, no presumed clustering
- Computational cost increases linearly
- Same complexity dealing with pairwise confinement interaction and flux-tube interaction



# Importance Sampling

In the Birth-death process:

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

In areas where the potential changes intensely, a tiny movement of the walker will lead to a drastic fluctuation of the population.

▷ *Importance sampling technique*

- Introduce importance function: $\psi_T(\boldsymbol{R})$, and sample $f(\boldsymbol{R},t) \equiv \Psi(\boldsymbol{R},t)\psi_T(\boldsymbol{R})$
- The $\psi_T(\boldsymbol{R})$ should be as close as possible to $\Psi_0(\boldsymbol{R})$
- Schrödinger equation with importance sampling

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

$$\boldsymbol{F}_i(\boldsymbol{R}) = 2\psi_T(\boldsymbol{R})^{-1}\nabla_{\boldsymbol{r}_i}\psi_T(\boldsymbol{R}) = \nabla \ln|\psi_T|^2, \quad E_L(\boldsymbol{R}) = \psi_T(\boldsymbol{R})^{-1}\widehat{H}\psi_T(\boldsymbol{R})$$

◆ Convection-diffusion equation: Salt in flowing water

- Drift term Green's function: $G_3(\boldsymbol{R},\boldsymbol{R}',t) = \delta\left(\boldsymbol{R}-\boldsymbol{R}'-\frac{\boldsymbol{F}(\boldsymbol{R})}{2m}t\right)$

Make a displacement: $\frac{\boldsymbol{F}(\boldsymbol{R})}{2m}\Delta\tau$

Drift

# Importance Sampling

- Two effects:
  1. Guides walkers to regions with higher probability density: drift force $\boldsymbol{F}_i(\boldsymbol{R}) = \nabla \ln |\psi_T|^2$
  2. Reduces the fluctuation of the population of walkers

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

$$n_r = e^{-\left(\frac{E_L(\boldsymbol{R})+E_L(\boldsymbol{R}')}{2} - E_R\right)\Delta\tau} \rightarrow 1$$

Hjorth-Jensen:2017gss, Gordillo:2020sgc

- In the practical simulation, the $\psi_T(\boldsymbol{R})$ is unknown beforehand

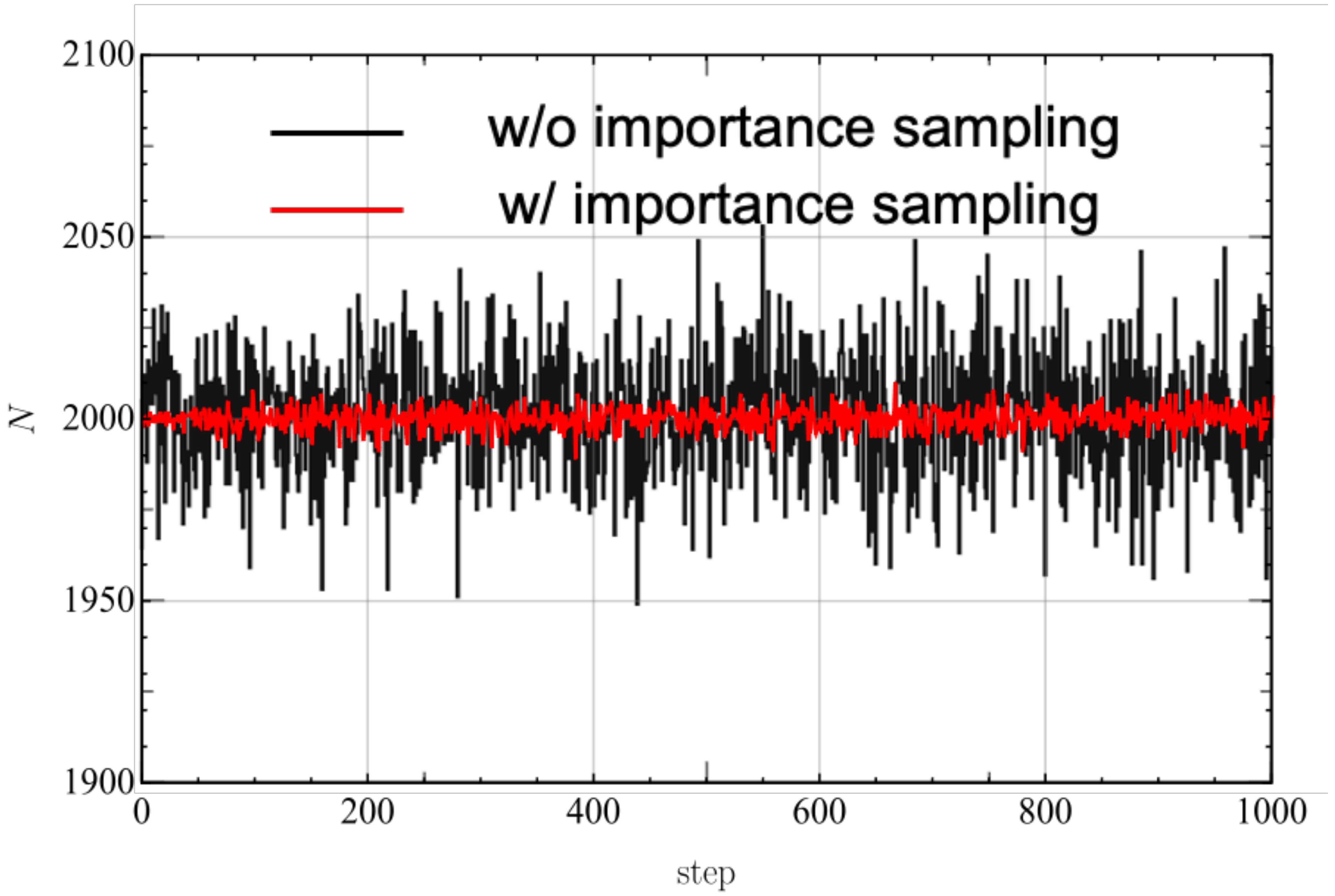
  In our calculation

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

- $a_{ij}$: adjustable constants, set to minimize fluctuation
- e.g. 1-d HO

$$H = -\frac{1}{2}\frac{\partial^2}{\partial x^2} + \frac{1}{2}x^2, E_0 = 0.5$$

With importance sampling, the fluctuation is reduced



# Application in baryons and tetraquark states

# Baryons

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

- Potential: AL1 and its revised version
- Two confinement scenarios ($\Delta$-type and Y-type)
- In variational method: It is hard to calculate the matrix elements of $V_{\rm conf}^{Y}$

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

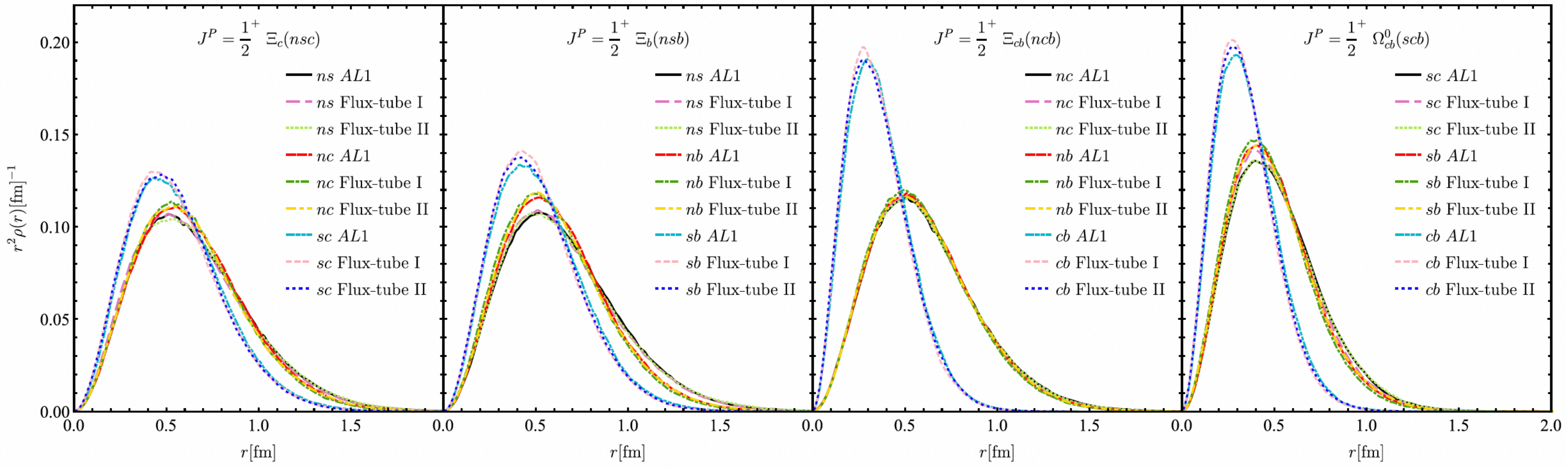
$$L_{min} = \left[ \frac{1}{2}(a^2 + b^2 + c^2) + \frac{\sqrt{3}}{2} \sqrt{(a+b+c)(-a+b+c)(a-b+c)(a+b-c)} \right]^{1/2}$$

Takahashi:2002bw

- In DMC: No need of integration, Steiner tree problem D. Smith, Algorithmica 7, 137 (1992)
- Coupling constants
  - $\sigma_{\Delta}$ from AL1 model
  - Flux tube-I: $\sigma_Y = \sigma_{\bar{q}q} = 2\sigma_{\Delta}$, Flux tube-II: fix $\sigma_Y$ from $\Omega(sss)$ mass, $\sigma_Y = 0.9204 \sigma_{\bar{q}q}$ Ma:2022vqf

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

- Results:



- Flux tube-II is more reliable
- For baryons it is hard to distinguish two confinement scenarios

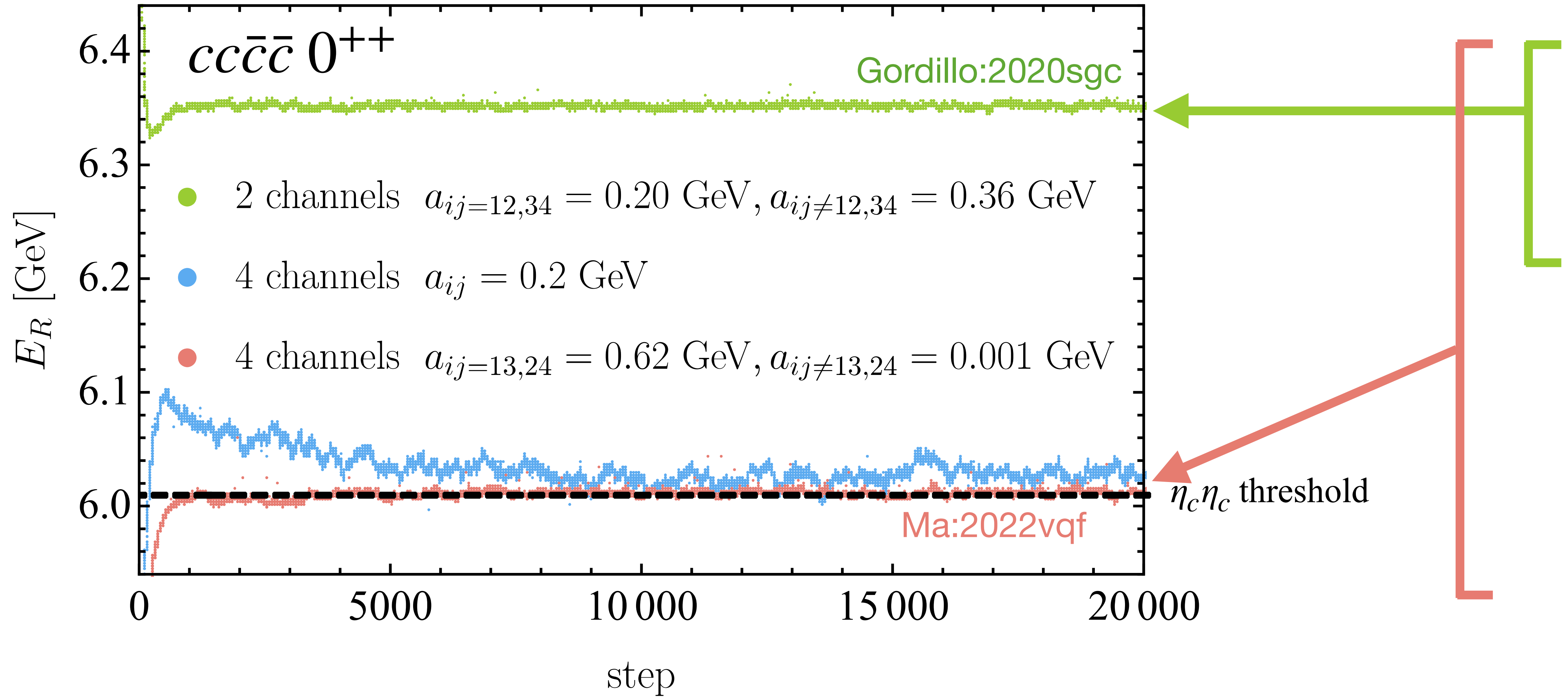
# DMC in quark models

- A lesson from nucleon calculation: proper configuration assignment
  - Single channel $|N\rangle_{\text{frac}} = \chi^S_{sf}(123)\psi^S(123)$ →not general enough
  - $|Ci\rangle = |Bi\rangle +$ even perm $(1,2,3)$,

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

| | AL1 | | | FT I | FT II | EXP |
|---|---|---|---|---|---|---|
| | DMC | VAR | Faddeev | | | |
| $\lvert N(123)\rangle_{\text{fac}}$ | 968 | 966 | 933 | 1059 | 975 | 939 |
| $\lvert N(123)\rangle_{\text{general}}$ | 930 | 930 | | 1019 | 936 | |

- $cc\bar{c}\bar{c}$ system
  - Cannot get the di-meson thresholds (real ground state for systems w/o bound states) Gordillo:2020sgc
  - Our advancement: including the extra two configuration channels Ma:2022vqf



$$
\begin{aligned}
|T1\rangle &= [(12)^{0_s}_{\bar{3}_c}(34)^{0_s}_{3_c}]^{0_s}_{1_c}\psi^{SS}_1(12;34),\\
|T2\rangle &= [(12)^{1_s}_{6_c}(34)^{1_s}_{\bar{6}_c}]^{0_s}_{1_c}\psi^{SS}_2(12;34),\\
|T3\rangle &= [(12)^{1_s}_{\bar{3}_c}(34)^{1_s}_{3_c}]^{0_s}_{1_c}\psi^{AA}_3(12;34),\\
|T4\rangle &= [(12)^{0_s}_{6_c}(34)^{0_s}_{\bar{6}_c}]^{0_s}_{1_c}\psi^{AA}_4(12;34).
\end{aligned}
$$

# DMC in quark models

- A lesson from nucleon calculation: proper configuration assignment
  - ◆ Single channel $|N\rangle_{\text{frac}} = \chi^S_{sf}(123)\psi^S(123)$ →not general enough
  - ◆ $|Ci\rangle = |Bi\rangle +$ even perm $(1,2,3)$,

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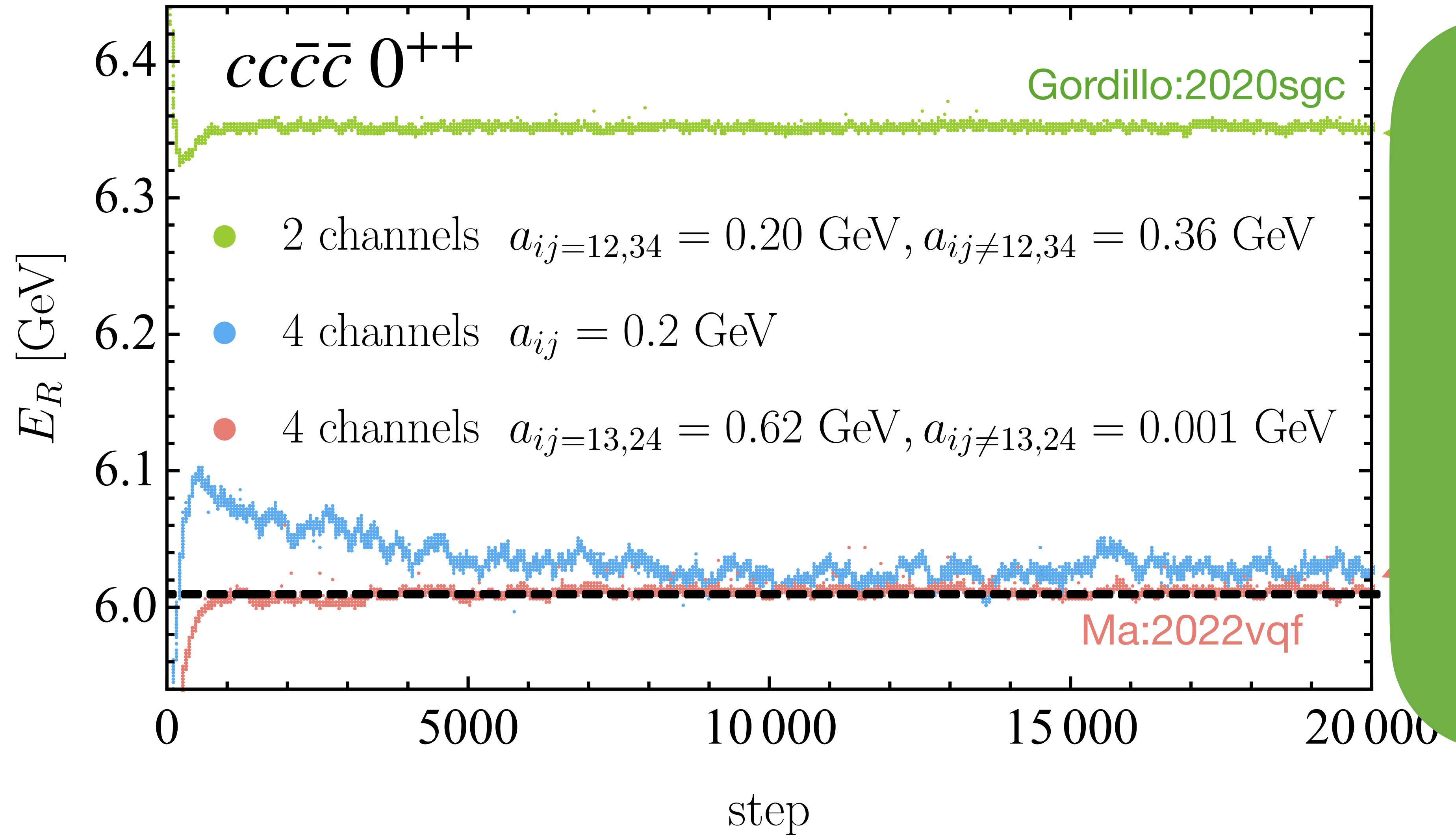


- ■ In variational method, it is hard to get the di-meson threshold without the di-meson clustering basis
- ■ In DMC, we get a di-meson type ground state without presuming such kind of clustering

# Double-heavy tetraquark

- Potential: Chiral quark models [Salamanca model (SLM)]
- Systems with bound state:

| $J^P$ | | $I$ | $E_{\text{th}}$ | $E$ | $\Delta E$ |
|---|---|---|---|---|---|
| $0^+$ | $bc\bar{n}\bar{n}$ | 0 | 7171 | 6986 | -185 |
| | $bc\bar{s}\bar{n}$ | $\frac{1}{2}$ | 7244 | 7243 | -1 |
| $1^+$ | $cc\bar{n}\bar{n}$ | 0 | 3915 | 3759 | -156 |
| | $bb\bar{n}\bar{n}$ | 0 | 10594 | 10249 | -345 |
| | $bb\bar{s}\bar{n}$ | $\frac{1}{2}$ | 10667 | 10653 | -14 |
| | $bc\bar{n}\bar{n}$ | 0 | 7215 | 7012 | -203 |
| | $bc\bar{s}\bar{n}$ | $\frac{1}{2}$ | 7291 | 7287 | -4 |

# Summary and outlook

- Improved DMC to give the di-meson threshold
- Recommended tetraquark bound states:

$$J^P = 1^+: \quad [cc\bar{n}\bar{n}]^{I=0},\ [bb\bar{n}\bar{n}]^{I=0},\ [bc\bar{n}\bar{n}]^{I=0},\ [bb\bar{s}\bar{n}],\ [bc\bar{s}\bar{n}]$$

$$J^P = 0^+: \quad [bc\bar{n}\bar{n}]^{I=0},\ [bc\bar{s}\bar{n}]$$

- Can be further improved: Auxiliary field diffusion Monte Carlo, fixed-node method
- Flux-tube confinement potentials for tetraquark states

Thanks for your attention!

# Backup

# Coupled-channel formalism

- Coupled-channel Schrödinger equation

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

$$-\frac{\partial\Psi_{\alpha'}}{\partial t}=\sum_{\alpha}\hat{H}_{\alpha'\alpha}\Psi_{\alpha}-E_{R}\Psi_{\alpha'}$$

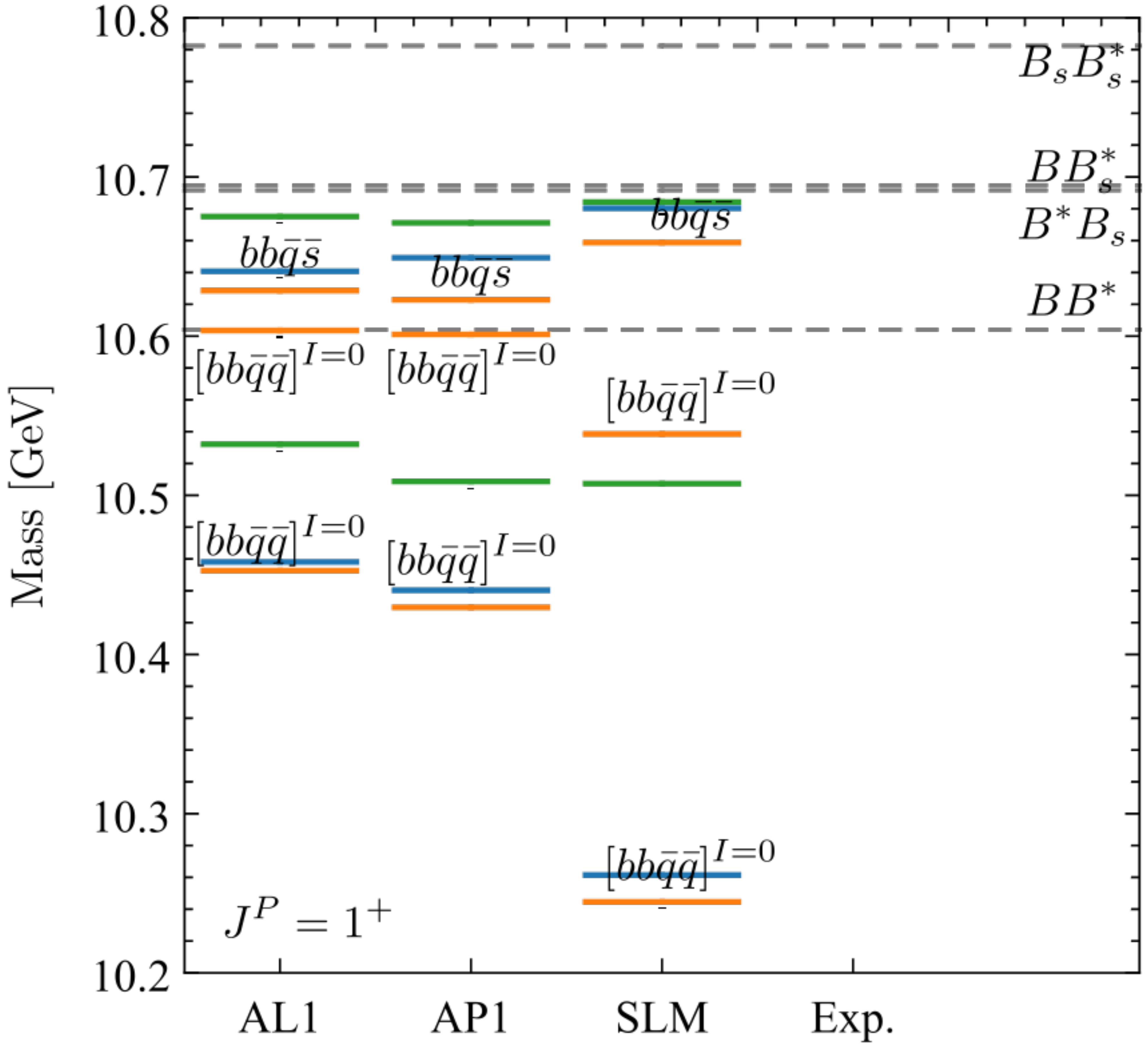
- Sample $\mathcal{F}(\boldsymbol{R},t)$

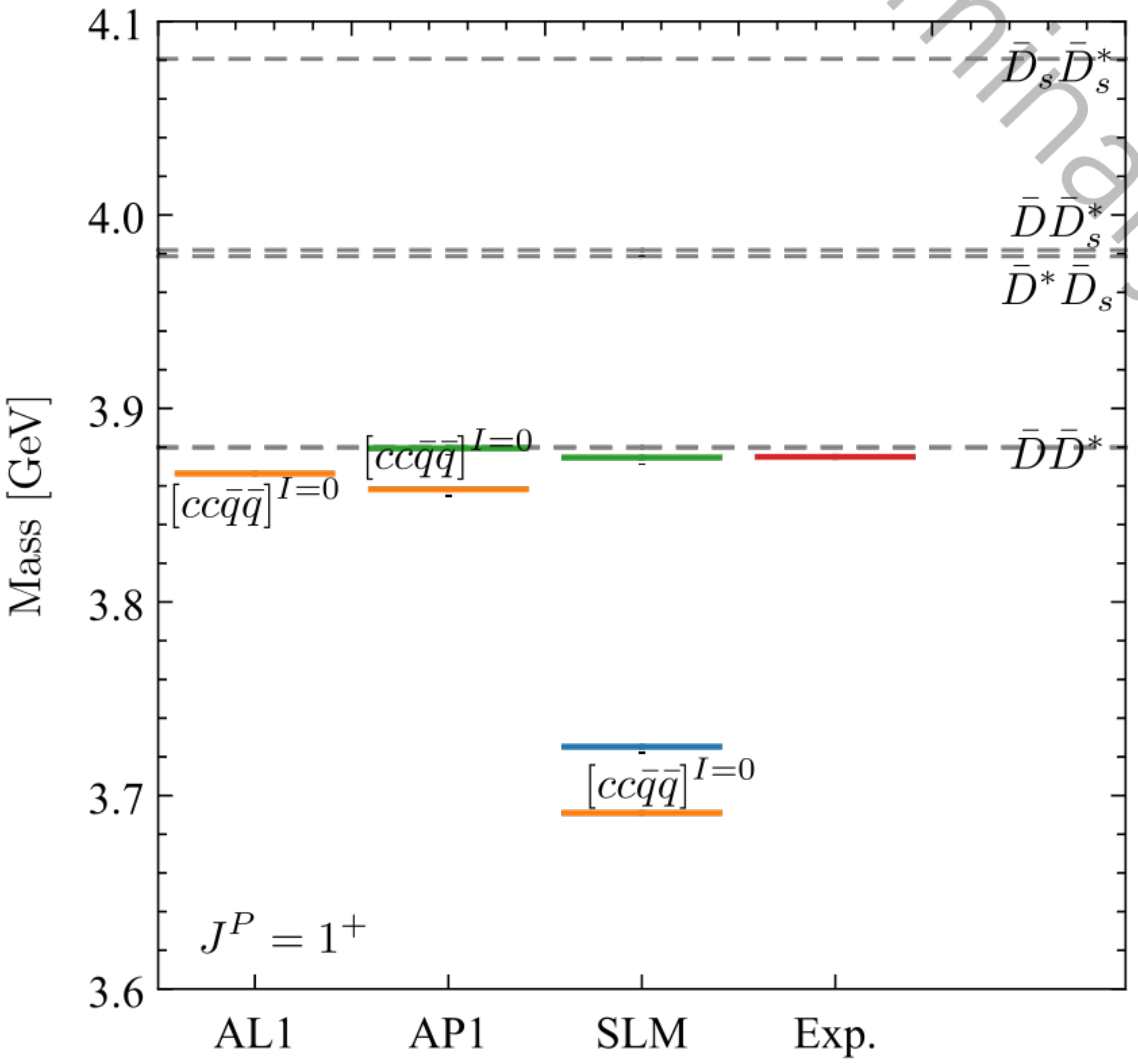
$$f_{\alpha}(\boldsymbol{R},t)\equiv\psi_{T}(\boldsymbol{R})\Psi_{\alpha}(\boldsymbol{R},t),$$

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

# Double-heavy tetraquark

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





# Systemic uncertainties

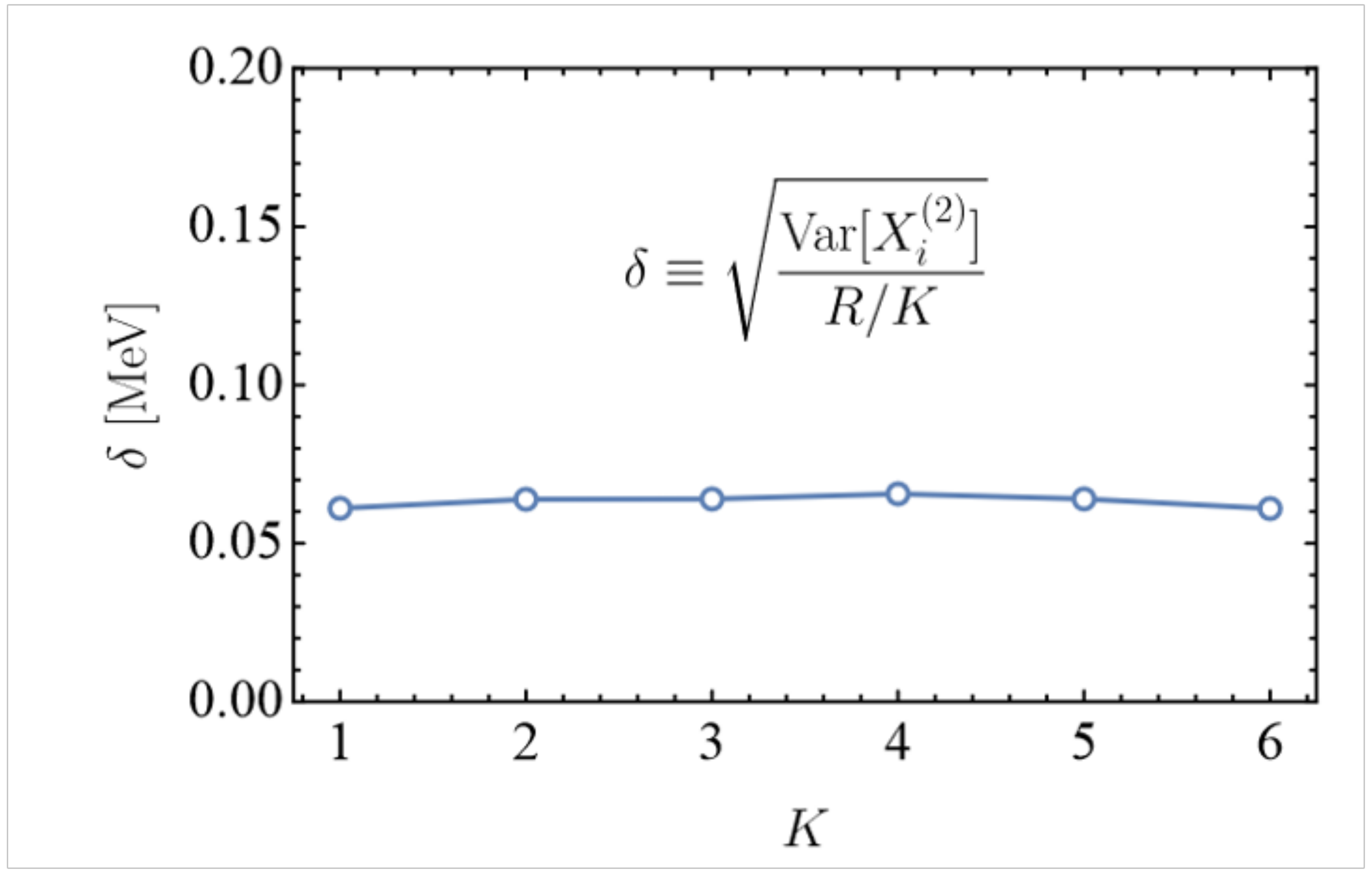
- Time-step uncertainty
- Walker number control uncertainty
- Choice of importance functions
- Fermion sign problem (Main problem)
  - The density of the walker is always positive
  - However, the wave functions can be negative
  - The present coupled channel strategy
  - Better choice: fixed-node method, 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

# Statistical uncertainties

- 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



# 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

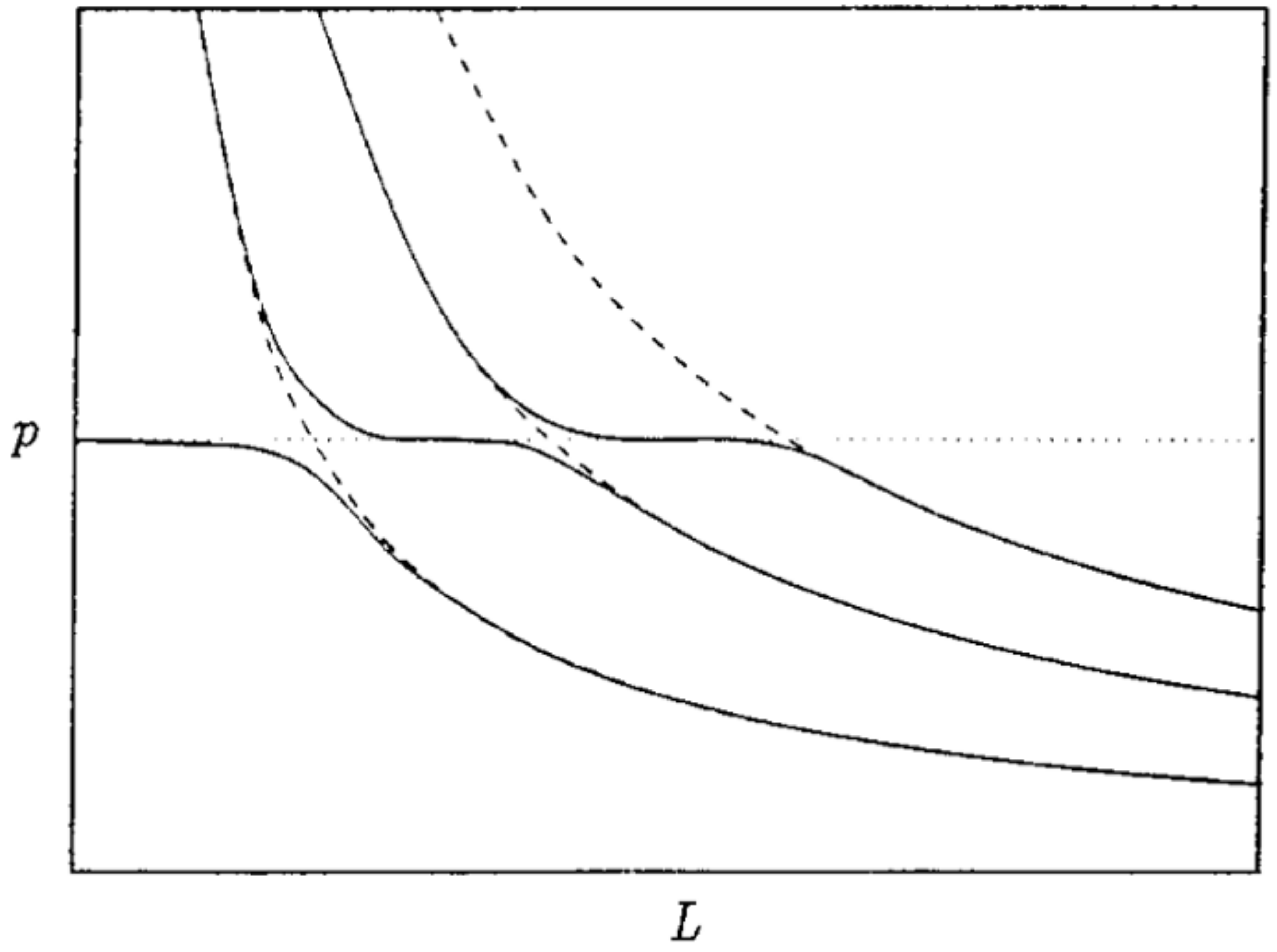


Figure 2: The finite volume spectrum of the free and the interacting model. Wiese:1988qy