



# Comparison between Variational Monte Carlo and Shell Model Calculations of Neutrinoless Double Beta Decay Matrix Elements in Light Nuclei

Xiaobao Wang

Wuhan, 2019

Collaborate with J.A. Carlson, A.C. Hayes, G.X. Dong,  
E. Mereghetti, S. Pastore, R.B. Wiringa

# Outline

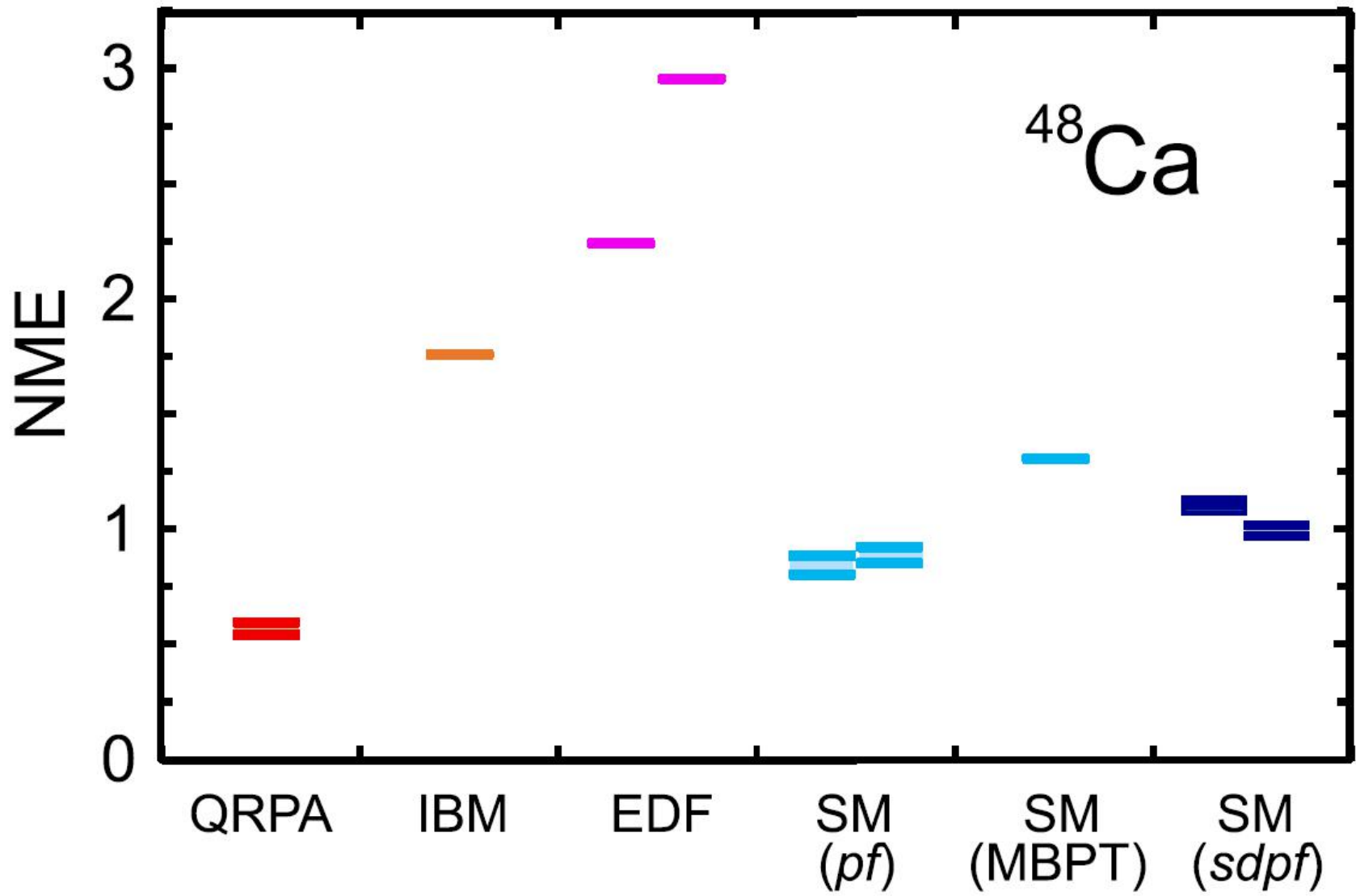
*Background*

*Normalizations: model space & radial wavefunctions*

*Short-range correlations*

*Results*

*Conclusion*



Large-Scale Shell-Model Analysis of the Neutrinoless  $\beta\beta$  Decay of  $^{48}\text{Ca}$   
Y. Iwata, N. Shimizu, T. Otsuka, Y. Utsuno, J. Menéndez, M. Honma, and T. Abe, PRL 116, 112502 (2016).

# Neutrinoless double- $\beta$ decay matrix elements in light nuclei

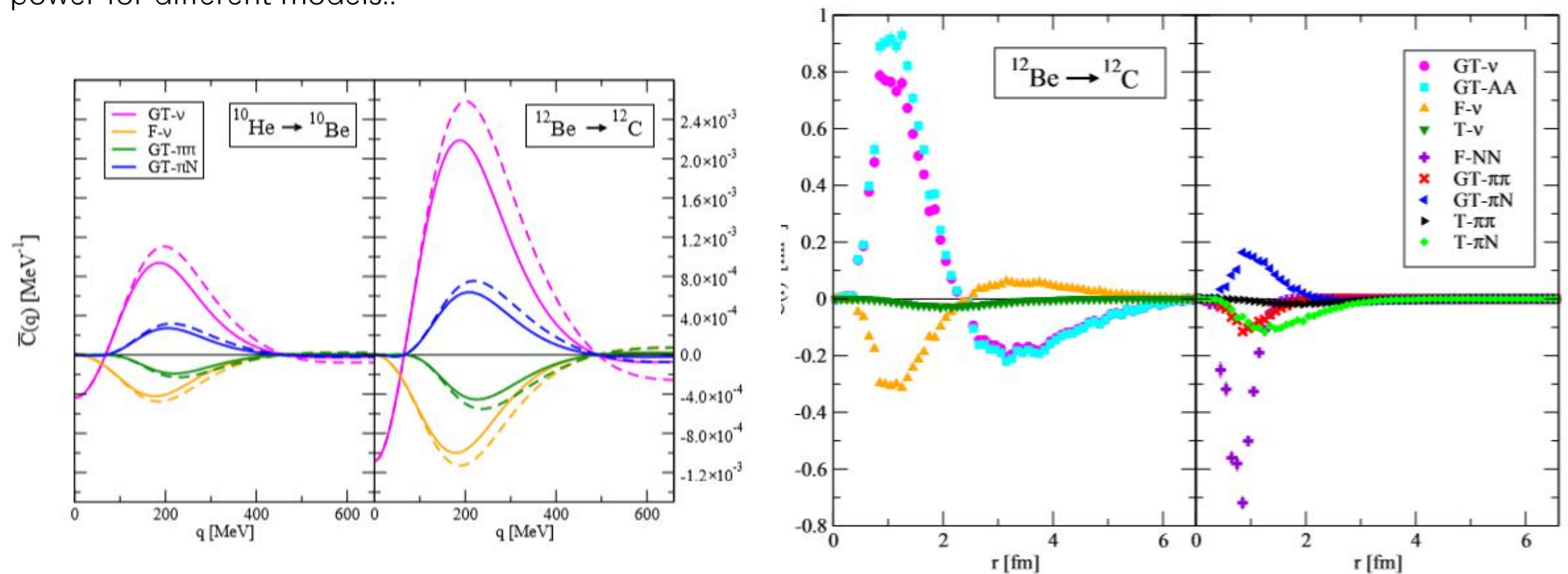
S. Pastore,<sup>1</sup> J. Carlson,<sup>1</sup> V. Cirigliano,<sup>1</sup> W. Dekens,<sup>1,2</sup> E. Mereghetti,<sup>1</sup> and R. B. Wiringa<sup>3</sup>

<sup>1</sup>Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA

<sup>2</sup>New Mexico Consortium, Los Alamos Research Park, Los Alamos, New Mexico 87544, USA

<sup>3</sup>Physics Division, Argonne National Laboratory, Argonne, Illinois 60439, USA

Provide benchmarks, to check the prediction power for different models..



**Neutrinoless double- $\beta$  decay matrix elements in light nuclei**S. Pastore,<sup>1</sup> J. Carlson,<sup>1</sup> V. Cirigliano,<sup>1</sup> W. Dekens,<sup>1,2</sup> E. Mereghetti,<sup>1</sup> and R. B. Wiringa<sup>3</sup><sup>1</sup>*Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA*<sup>2</sup>*New Mexico Consortium, Los Alamos Research Park, Los Alamos, New Mexico 87544, USA*<sup>3</sup>*Physics Division, Argonne National Laboratory, Argonne, Illinois 60439, USA*

assume a functional form for the variational wavefunction (*trial wavefunction*) that depends on a set of parameters  $\{p\}$

*variational theorem*: the expectation value of the Hamiltonian computed on a trial wavefunction is always an upper bound to the true ground state energy of the system

$$\frac{\langle \psi_T(\alpha, \{p\}) | H | \psi_T(\alpha, \{p\}) \rangle}{\langle \psi_T(\alpha, \{p\}) | \psi_T(\alpha, \{p\}) \rangle} = E_T(\{p\}) \geq E_0$$

↘ stochastic integration, M(RT)<sup>2</sup> algorithm

VMC implies a minimization of  $E_T(\{p\})$  with respect to the parameters  $\{p\}$  in order to find the optimal trial wavefunction that better approximates the ground state wavefunction

Neutrinoless double- $\beta$  decay matrix elements in light nuclei

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$$E_V = \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle} \geq E_0$$

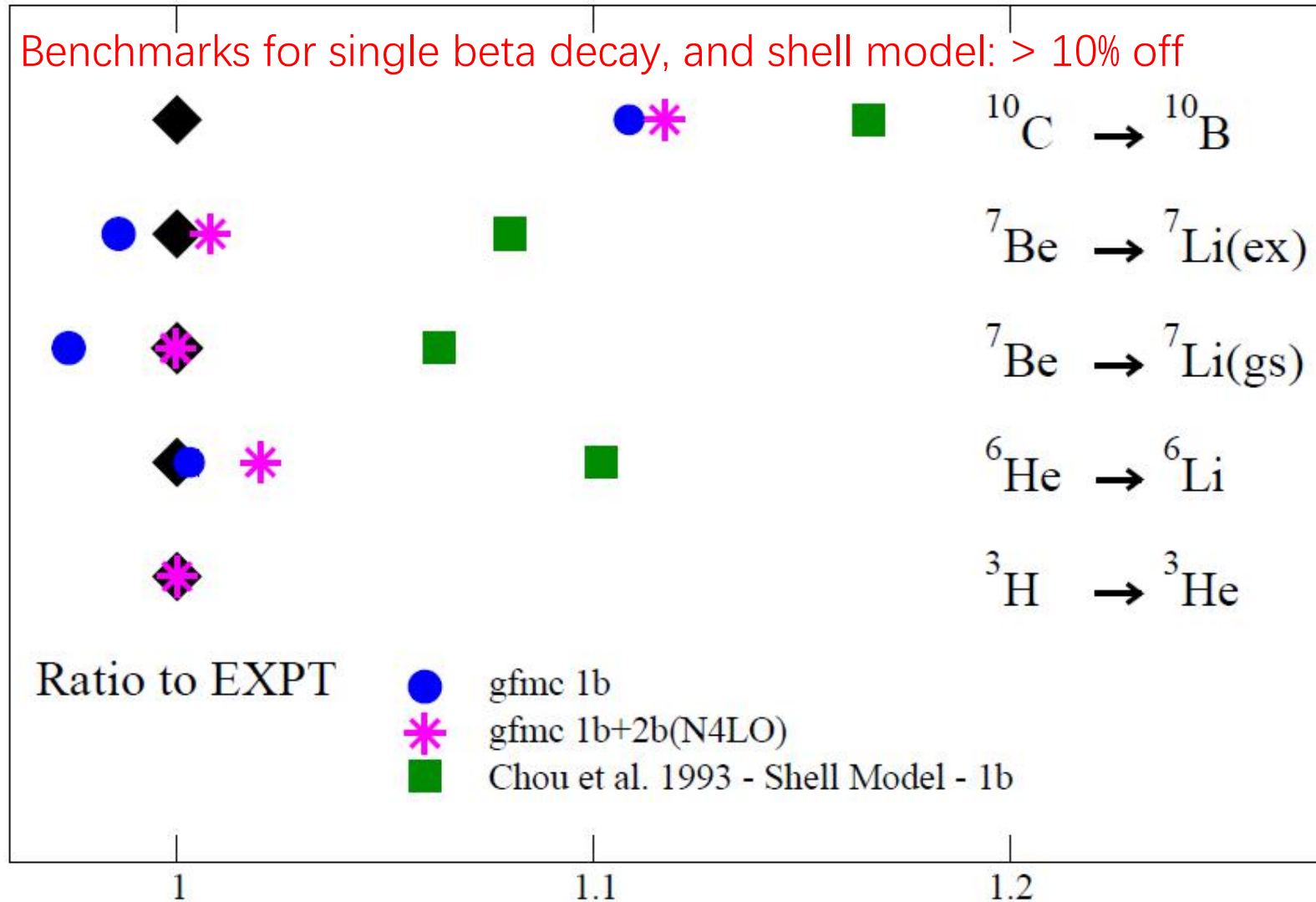
$$H = -\frac{\hbar^2}{2m} \sum_i \nabla_i^2 + \sum_{i < j} v_{ij} + \sum_{i < j < k} V_{ijk}.$$

$$\begin{aligned} \langle RS | \Psi \rangle &= \langle RS | \prod_{i < j} f_{ij}^1 \prod_{i < j < k} f_{ijk}^{3c} \\ &\times \left[ \mathbb{1} + \sum_{i < j} \sum_{p=2}^6 f_{ij}^p \mathcal{O}_{ij}^p f_{ij}^{3p} + \sum_{i < j < k} U_{ijk} \right] |\Phi \rangle_{J^\pi, T}, \end{aligned}$$

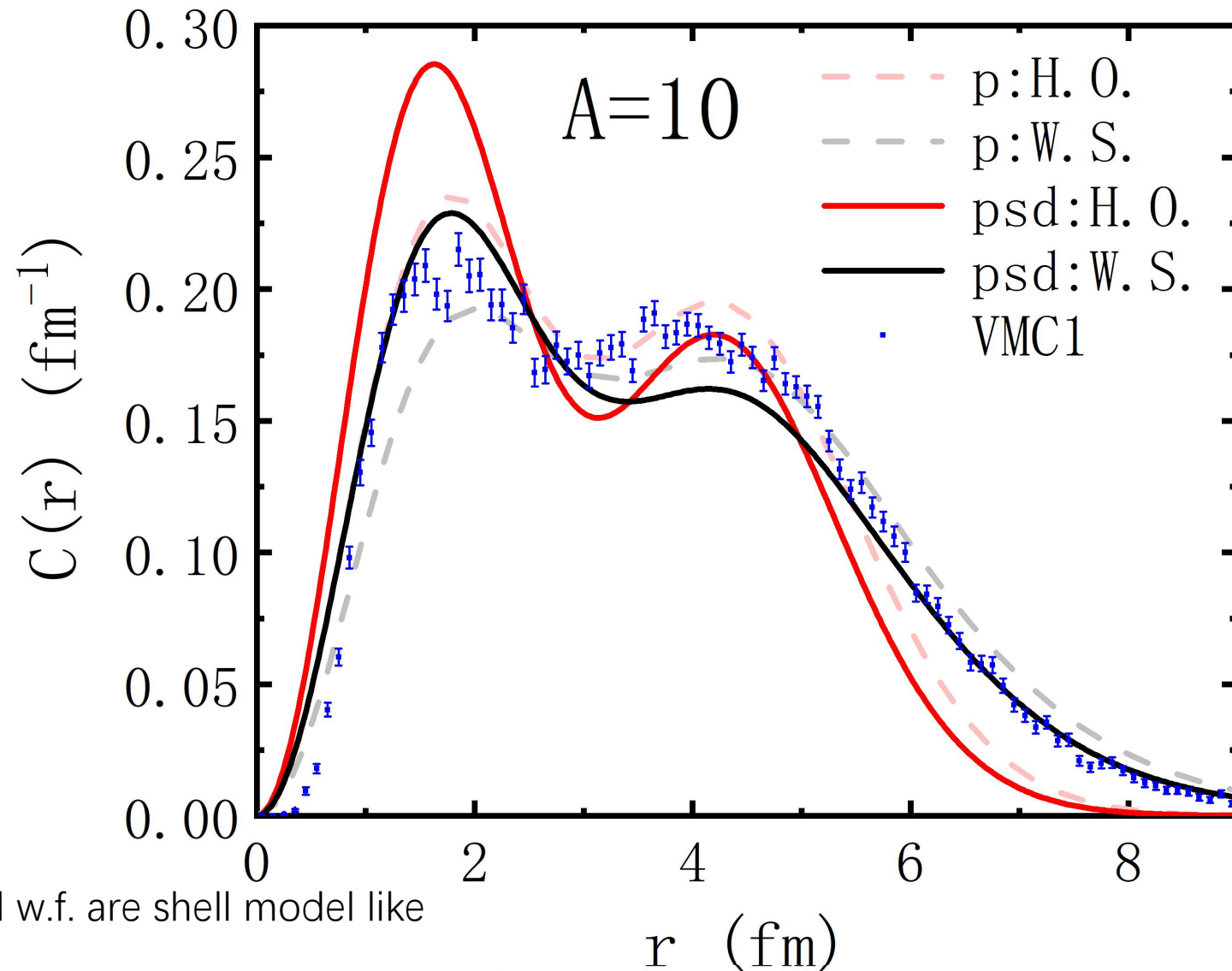


Quantum Monte Carlo calculations of weak transitions in  $A=6-10$  nucleiS. Pastore<sup>a</sup>, A. Baroni<sup>b</sup>, J. Carlson<sup>a</sup>, S. Gandolfi<sup>a</sup>, Steven C. Pieper<sup>d</sup>, R. Schiavilla<sup>b,c</sup>, and R.B. Wiringa<sup>d</sup>

Phys. Rev. C97, 022501(R) (2018)



# Norm Matrix Element $\langle i | \mathbf{1} | \text{tau} + \text{tau} + | f \rangle$



Shell model, VMC, and other models, have to give **the same value**.  
But you can see the discrepancies, explicitly..

Here, there are different “choices” made for shell model:

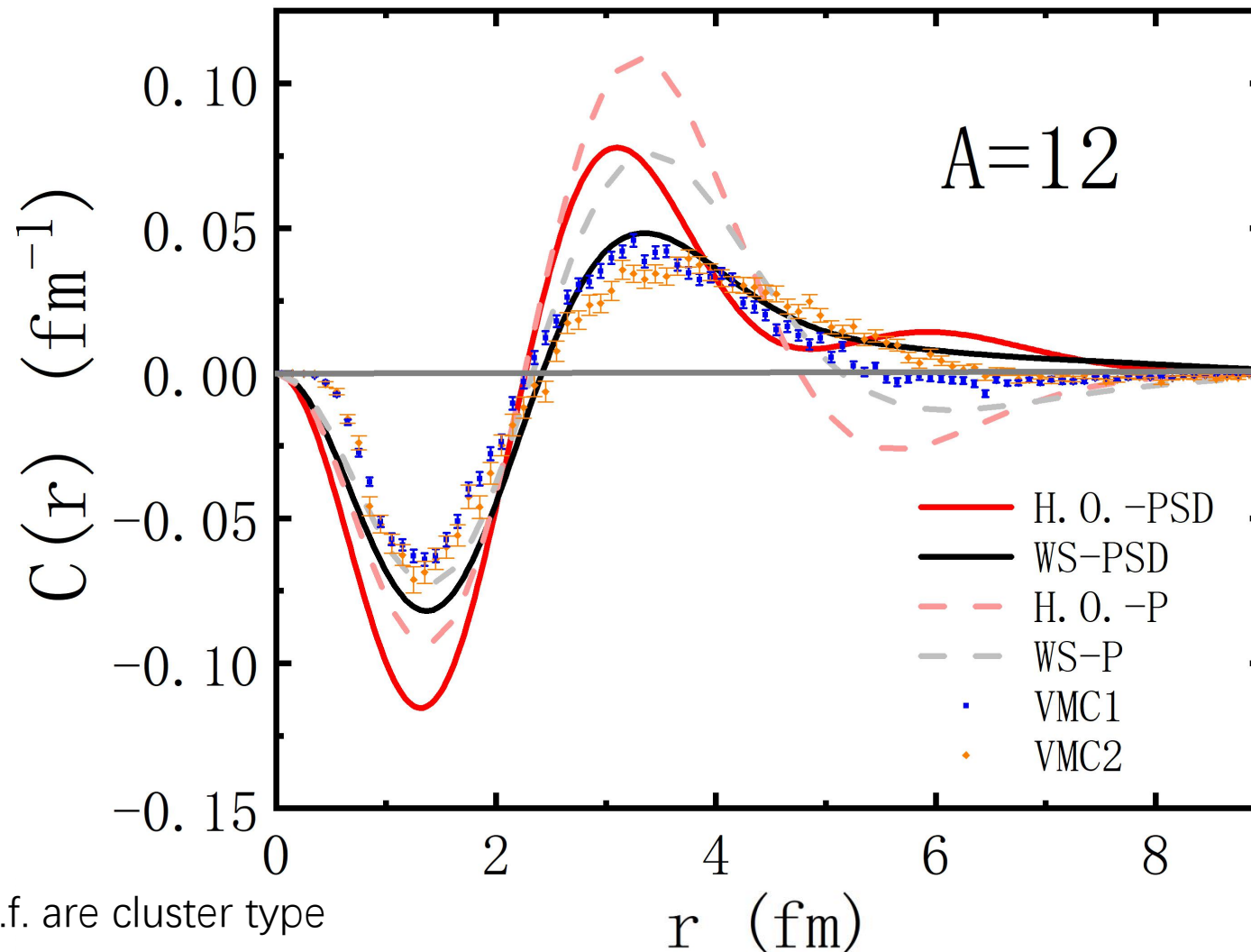
- 1) **model space**;
- 2) **radial wavefunctions**.

VMC1: variational w.f. are shell model like

$$A=10 : \langle \text{Be10\_g.s., } T=1 | \mathbf{1} | \text{C10\_g.s., } T=1 \rangle = 1.000$$



# Norm Matrix Element $\langle i | \mathbf{1} \text{ tau+tau+} | f \rangle$



Shell model, VMC, and other models, have to give **the same value**.

But you can see the discrepancies, explicitly..

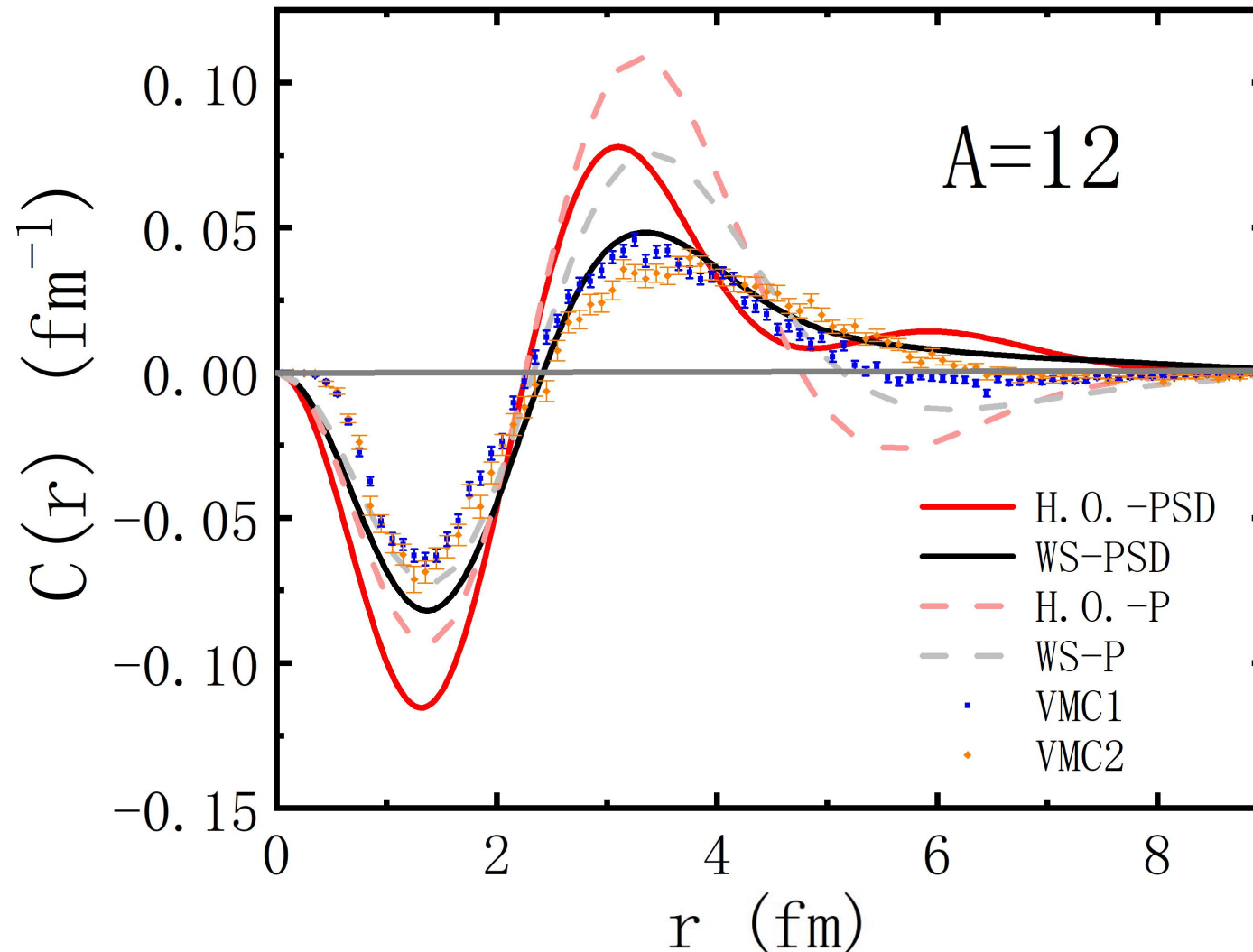
Here, there are different “choices” made for shell model:

- 1) **model space**;
- 2) **radial wavefunctions**.

VMC2: variational w.f. are cluster type

$$A=12: \langle \text{Be12\_g.s., } T=2 | \mathbf{1} | \text{C12\_g.s., } T=0 \rangle = \mathbf{0.000}$$

## Choice of model space



Different model space, has different nodes.

Of course, extended model space used for shell model gives better agreements with VMC method.

$$A=12: \langle \text{Be12}_{\text{g.s.}}, T=2 | 1 | \text{C12}_{\text{g.s.}}, T=0 \rangle = \mathbf{0.000}$$

# Choice of radial wave functions

The distributions of TBME for  $J_0 = 0$  ( $A=12$ )

H.O.: chosen most frequently, easy to use.

SHF: from Skyrme-HF

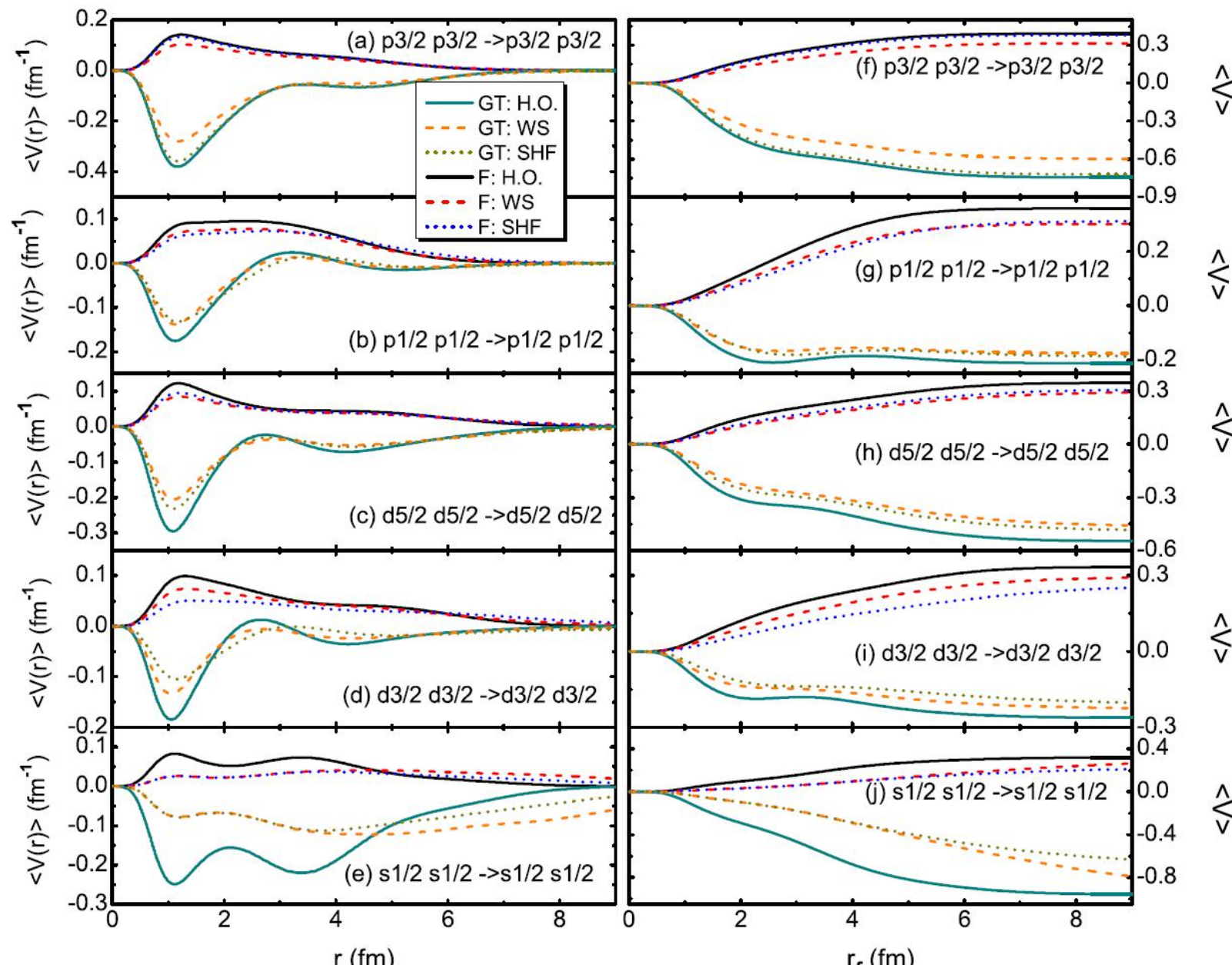
WS: from Woods-Saxon potential

H.O.: more concentrated, Larger overlap, decay faster against  $r$ .

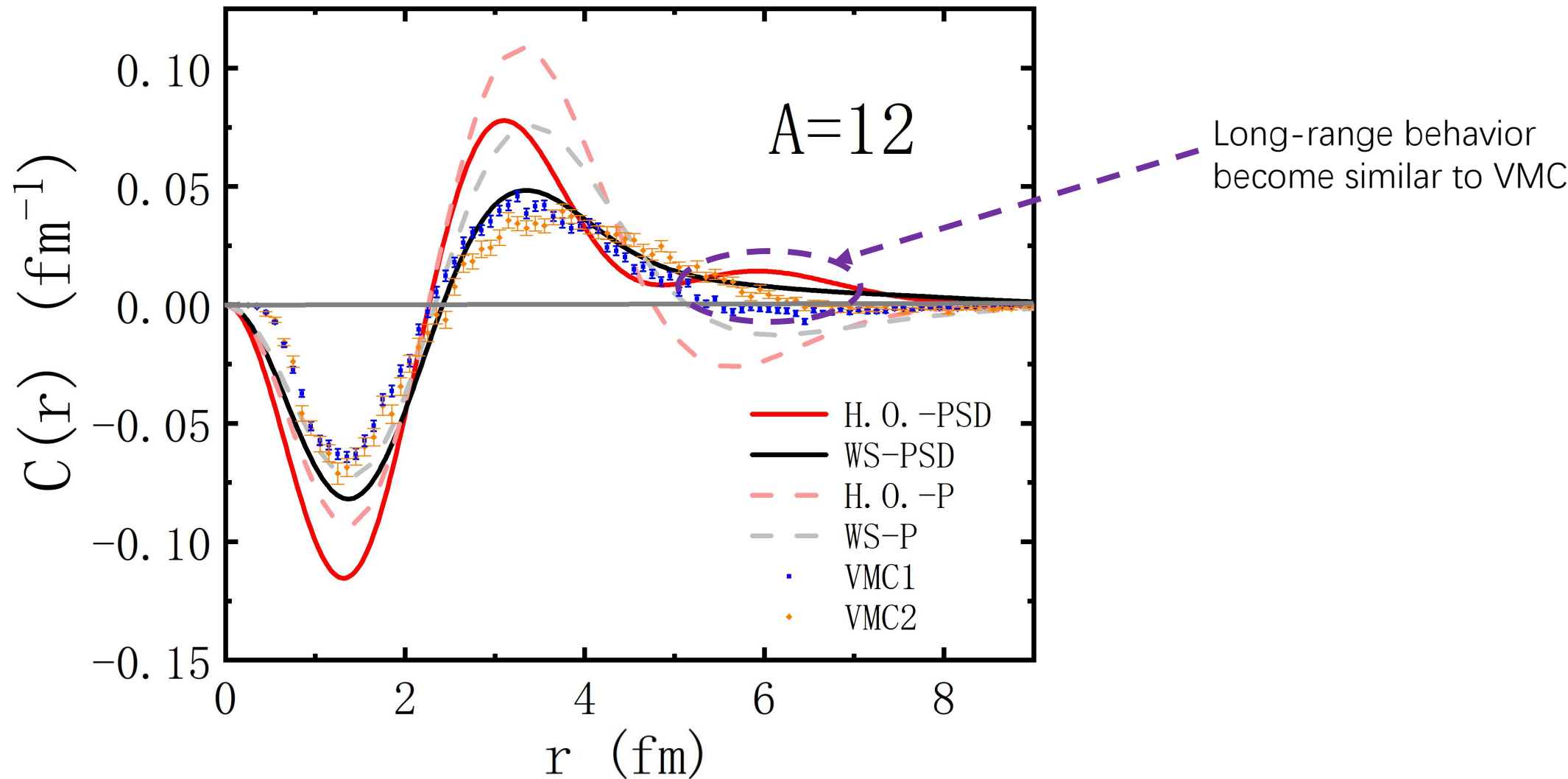
SHF/WS: smaller overlaps, Correct the asymptotic behavior of H.O.

integrated matrix element,  $\int_0^{r_f} C(r)dr$

as a function of the upper limit of the radial integral



# Choice of radial wave functions



$A=12: \langle \text{Be12\_g.s., } T=2 \mid 1 \mid \text{C12\_g.s., } T=0 \rangle = \mathbf{0.000}$



## Operators for 0vDB NMEs:

$$V_\nu = m_\pi \tau_a^+ \tau_b^+ \left( \mathbf{1} \times \mathbf{1} V_F^\nu(z) - g_A^2 \boldsymbol{\sigma}_a \cdot \boldsymbol{\sigma}_b V_{GT}^\nu(z) - g_A^2 S_{ab} V_T^\nu(z) \right)$$

$$M_{GT}^\beta = (4\pi R_A) \sigma_1 \cdot \sigma_2 V_{GT}^\beta(r_{12}) \tau_1^+ \tau_2^+ ,$$

$$M_F^\beta = (4\pi R_A) V_F^\beta(r_{12}) ,$$

$$M_T^\beta = (4\pi R_A) [3 (\sigma_1 \cdot \hat{r}) (\sigma_2 \cdot \hat{r}) - \sigma_1 \cdot \sigma_2] V_T^\beta(r_{12})$$

$R_A = 1.2A^{1/3}$  fm is the nuclear radius

**Leading terms:**

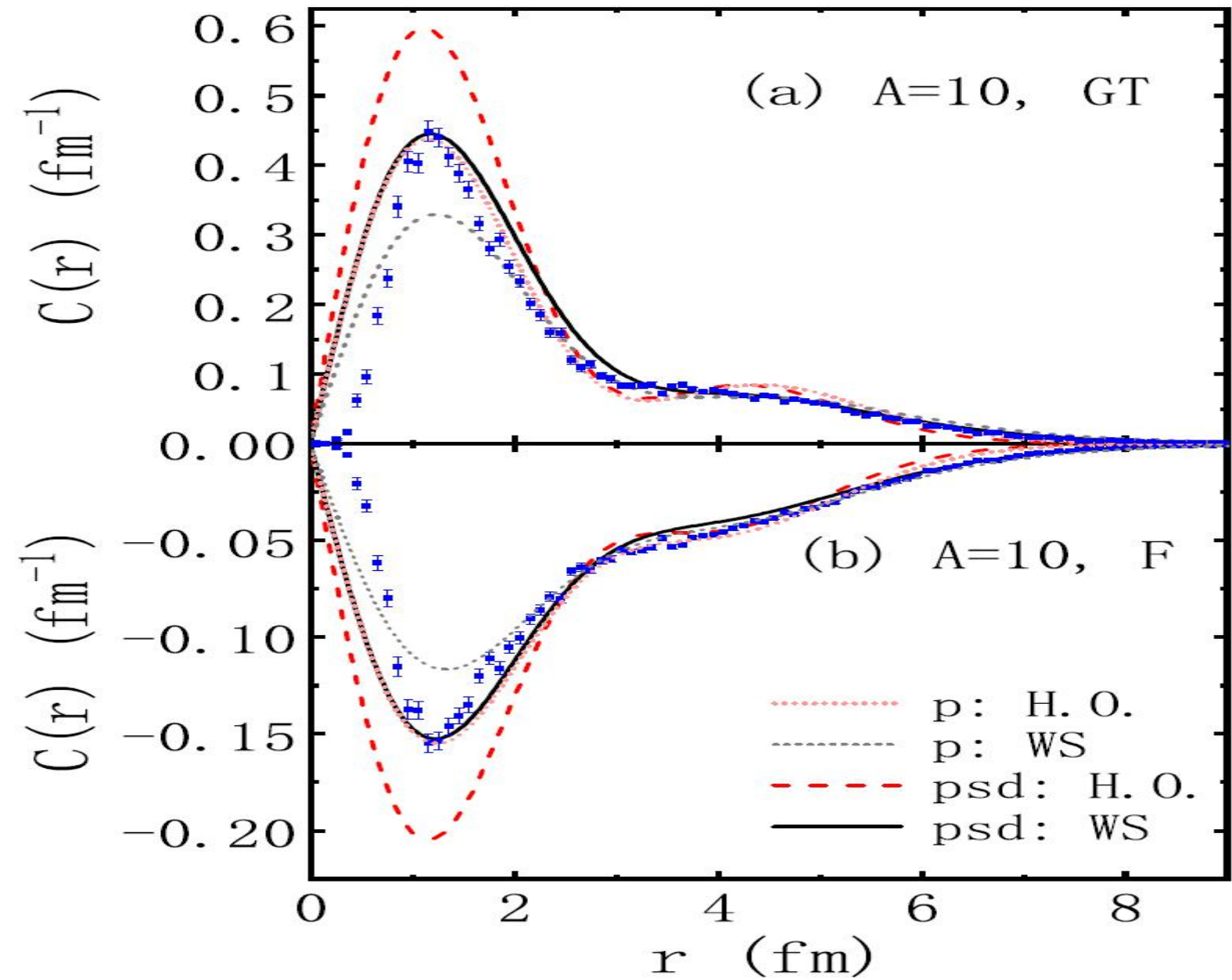
$$V_{F,\nu}(z) = \frac{1}{4\pi z}$$

$$V_{GT,AA}(z) = \frac{1}{4\pi z}$$

$$V_{GT,\nu}(z) = V_{GT,AA}(z) + V_{GT,AP}(z) + V_{GT,PP}(z) + V_{GT,MM}(z)$$

Operator **1/r**

A=10, Delta T =0



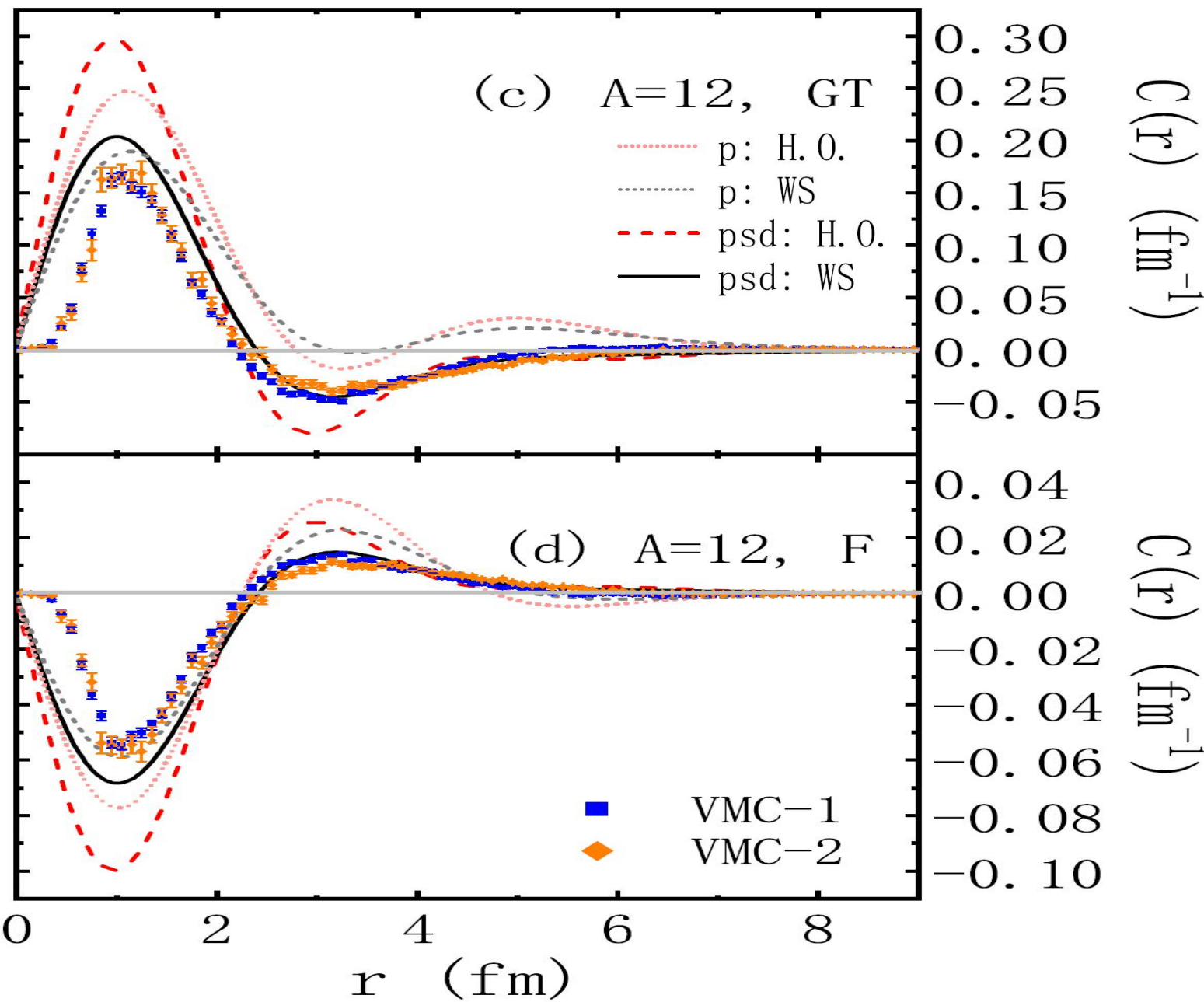
	$^{10}\text{Be}(0_1^+) \rightarrow ^{10}\text{C}(0_1^+)$	
	F	GT
VMC-1	-1.001(40)	2.273(91)
VMC-2	—	—
SM <sub>H.O.</sub> (w/o SRC, <i>p</i> )	-1.127	2.616
SM <sub>WS</sub> (w/o SRC, <i>p</i> )	-0.980	2.269
SM <sub>H.O.</sub> (w/o SRC, <i>psd</i> )	-1.274	3.228
SM <sub>WS</sub> (w/o SRC, <i>psd</i> )	-1.100	2.783

**p -> psd**  
Larger model space → more correlations → matrix elements become larger

**H.O. -> WS**  
W.S. r.w.f is less concentrated than H.O. ones → reduced matrix elements



Operator  $1/r$



$A=12$ ,  $\Delta T = 2$

		$^{12}\text{Be}(0_1^+) \rightarrow ^{12}\text{C}(0_1^+)$	
		F	GT
VMC-1		-0.100(4)	0.257(10)
VMC-2		-0.113(5)	0.274(11)
SM <sub>H.O.</sub> (w/o SRC, $p$ )		-0.183	1.228
SM <sub>WS</sub> (w/o SRC, $p$ )		-0.147	1.023
SM <sub>H.O.</sub> (w/o SRC, $psd$ )		-0.271	0.770
SM <sub>WS</sub> (w/o SRC, $psd$ )		-0.198	0.570

$p \rightarrow psd$   
Larger model space  $\rightarrow$  more correlations  $\rightarrow$  matrix elements can be reduced (remind: canceling effect for the normalizations)  
 $H.O. \rightarrow WS$   
W.S. r.w.f is less concentrated than H.O. ones  $\rightarrow$  reduced matrix elements

## More correlations, reduced matrix element

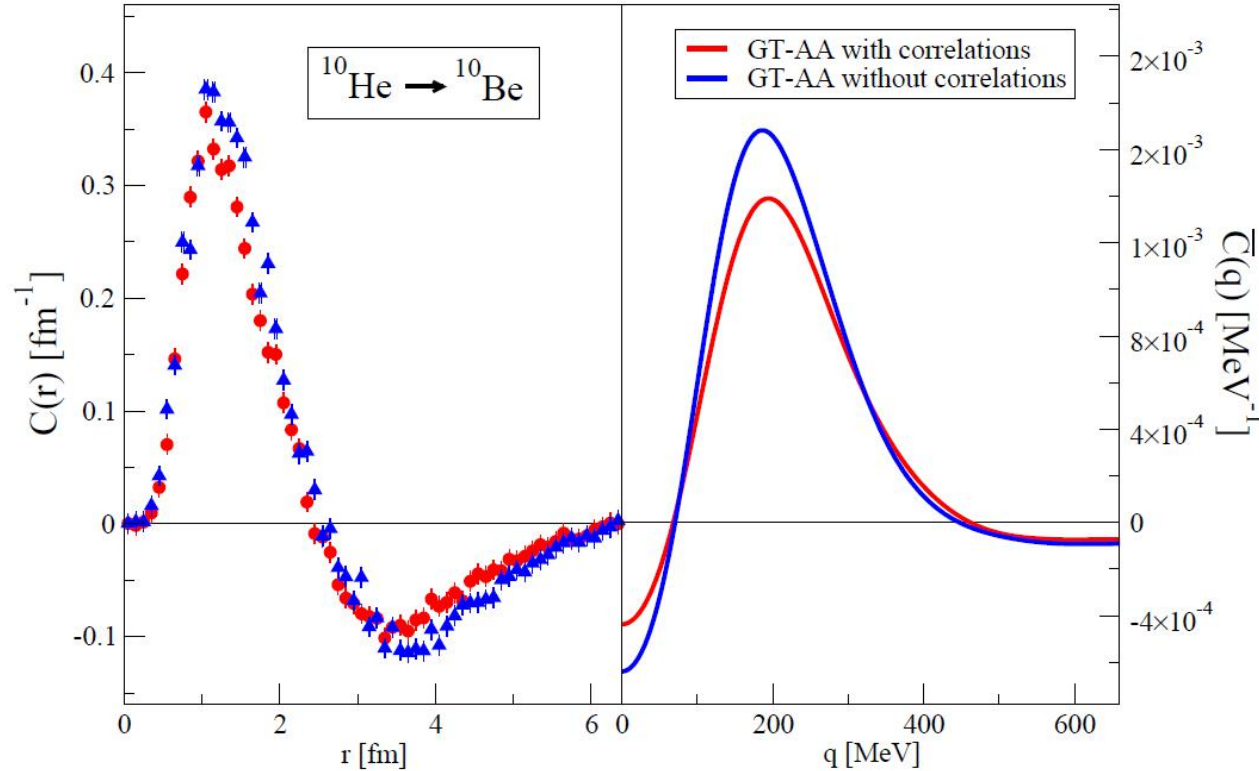
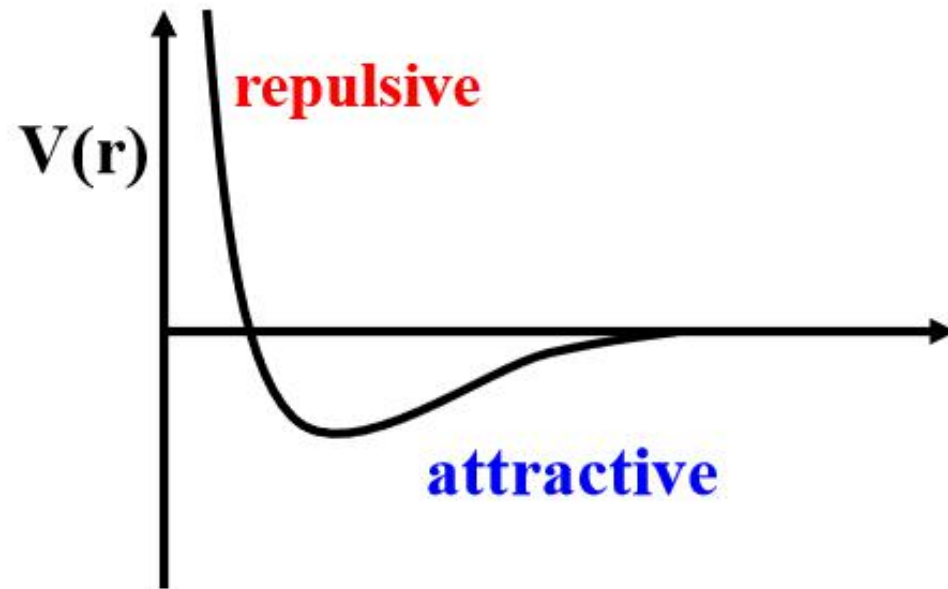
Neutrinoless double- $\beta$  decay matrix elements in light nucleiS. Pastore,<sup>1</sup> J. Carlson,<sup>1</sup> V. Cirigliano,<sup>1</sup> W. Dekens,<sup>1,2</sup> E. Mereghetti,<sup>1</sup> and R. B. Wiringa<sup>3</sup><sup>1</sup>Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA<sup>2</sup>New Mexico Consortium, Los Alamos Research Park, Los Alamos, New Mexico 87544, USA<sup>3</sup>Physics Division, Argonne National Laboratory, Argonne, Illinois 60439, USA

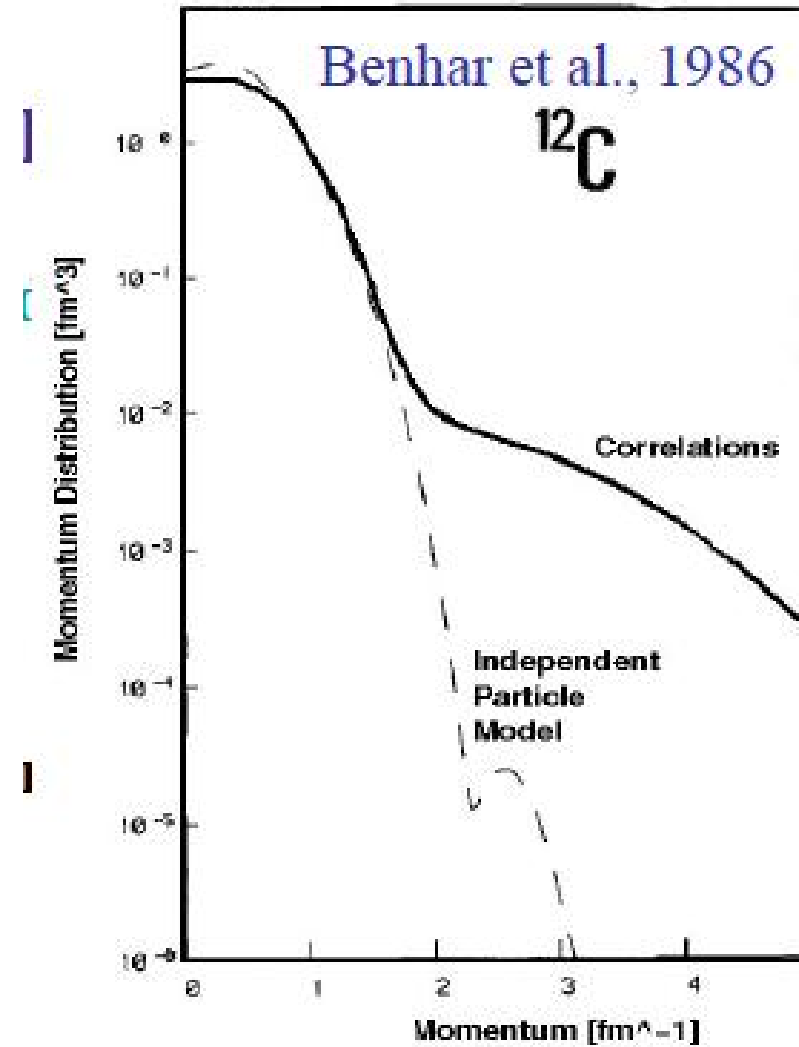
FIG. 6. The left (right) panel shows the GT-AA distribution in  $r$ -space ( $q$ -space) for the  $^{10}\text{He} \rightarrow ^{10}\text{Be}$  transition, with and without “one-pion-exchange-like” correlations in the nuclear wave functions. See text for explanation.

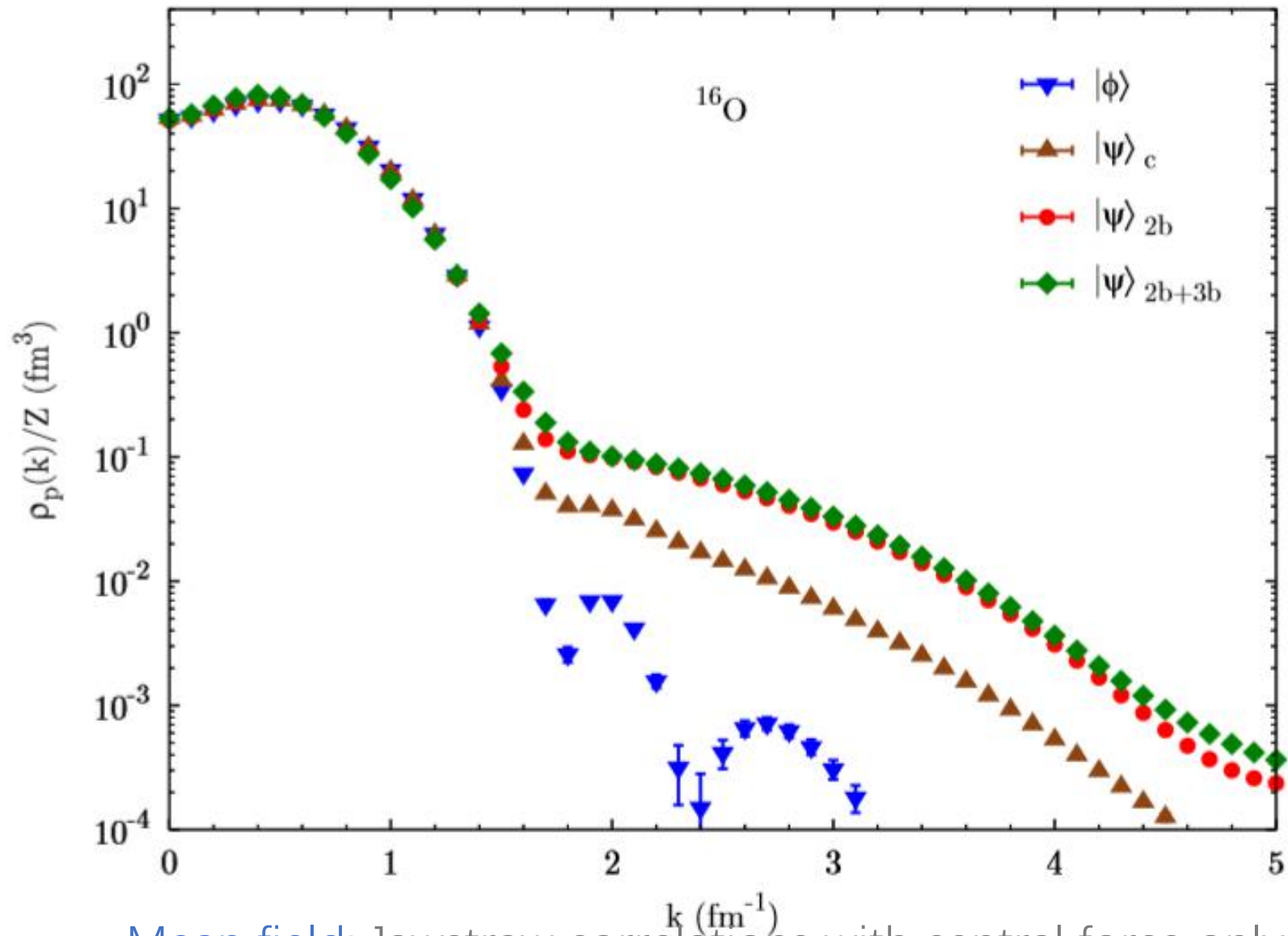
# Short range correlations: “disaster” for shell model?

The N-N interaction is attractive at a typical distance of 2 fm, but highly repulsive at distances  $< 0.5$  fm.



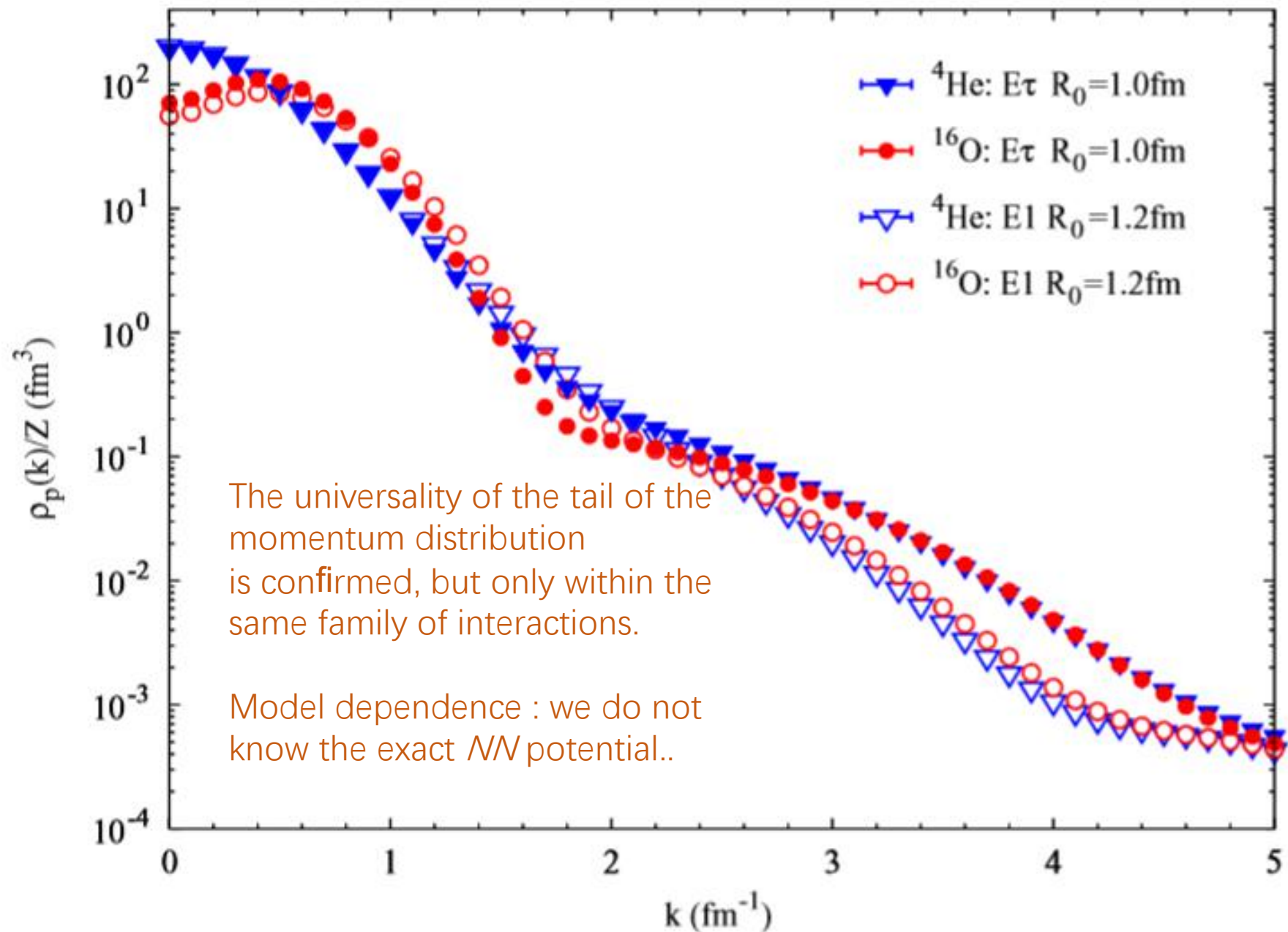
Short range repulsion and High momentum tail





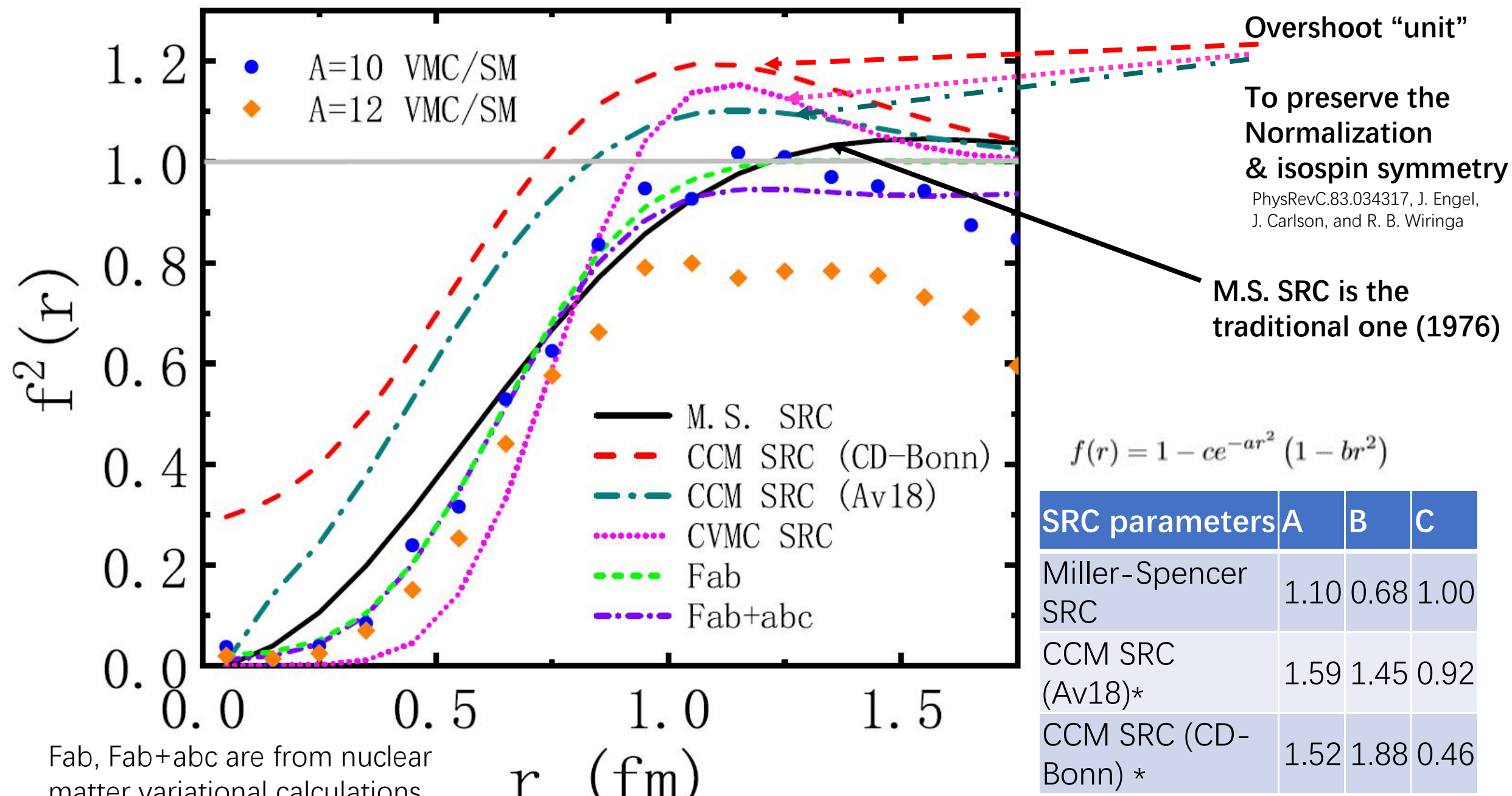
Mean field; Jawstraw correlations with central force only;

Full two body; 2+3 bd force



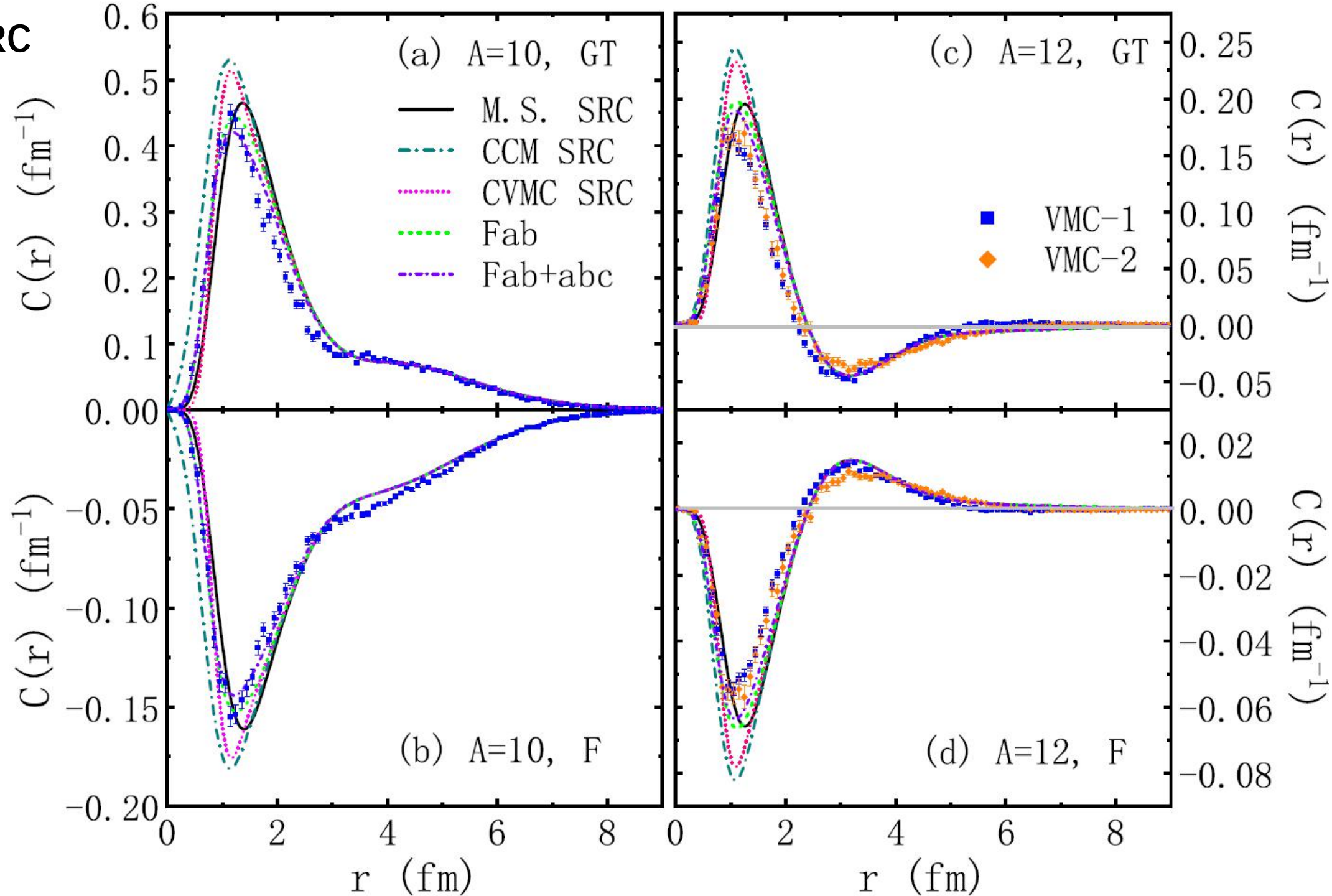


# A collection of short range correlations:





With SRC



# Results

	$^{10}\text{Be}(0_1^+) \rightarrow ^{10}\text{C}(0_1^+)$		$^{12}\text{Be}(0_1^+) \rightarrow ^{12}\text{C}(0_1^+)$	
	F	GT	F	GT
VMC-1	-1.001(40)	2.273(91)	-0.100(4)	0.257(10)
VMC-2	—	—	-0.113(5)	0.274(11)
$\text{SM}_{\text{WS}}(\text{M.S. SRC}, \textit{psd})$	-0.967	2.381	-0.122	0.342
$\text{SM}_{\text{WS}}(\text{CCM SRC}, \textit{psd})$	-1.069	2.683	-0.175	0.499
$\text{SM}_{\text{WS}}(\text{CVMC SRC}, \textit{psd})$	-0.992	2.457	-0.141	0.398
$\text{SM}_{\text{WS}}(\text{Fab}, \textit{psd})$	-0.988	2.449	-0.138	0.388
$\text{SM}_{\text{WS}}(\text{Fab}+\text{abc}, \textit{psd})$	-0.957	2.362	-0.128	0.361

For details:  
*X.B. Wang, et. al., Physics Letters B 798 (2019) 134974*

# Conclusions from the study of light nuclei

- 1. The use of H.O. **radial wave functions** will likely lead
- to an overestimate of matrix elements.
- 2. Limited size **model space** calculations could affect the magnitude of the predicted  $0\nu\beta\beta$  matrix elements, particularly for calculations constrained to a single shell.
- 3. The inclusion of a **SRC** function is needed.
- The best choice for this function requires further study.

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THANKS!

## Choice of model space

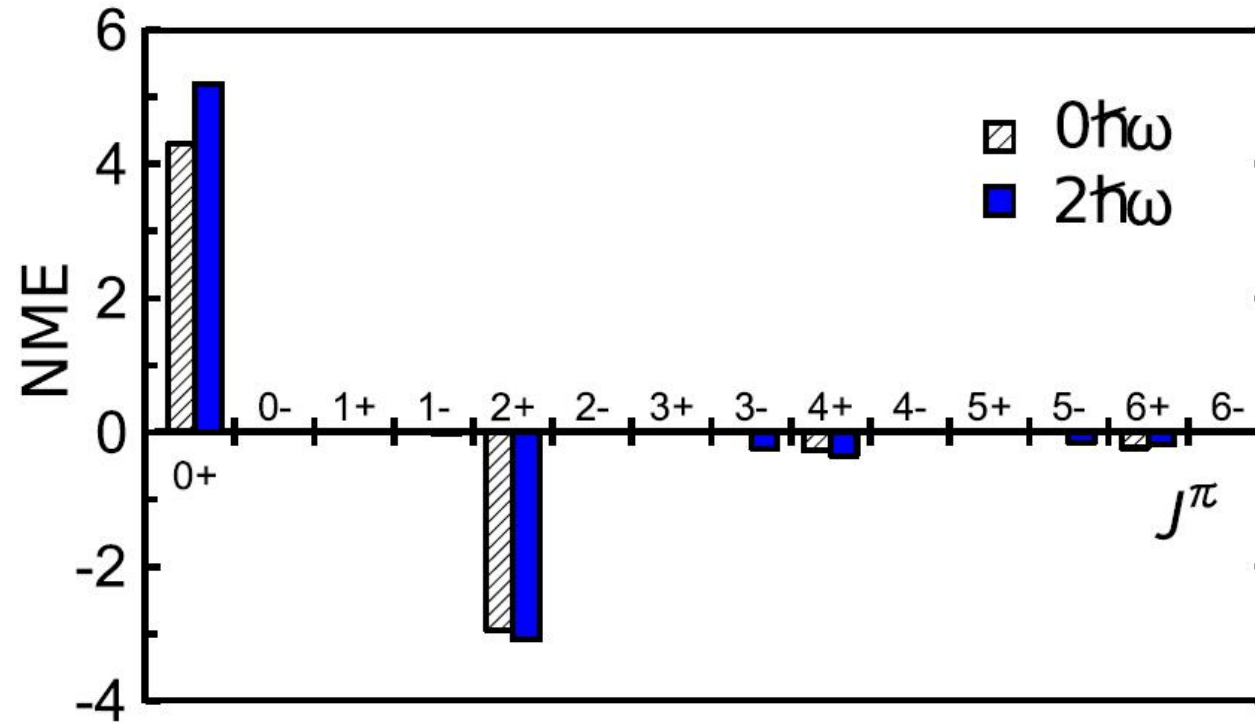
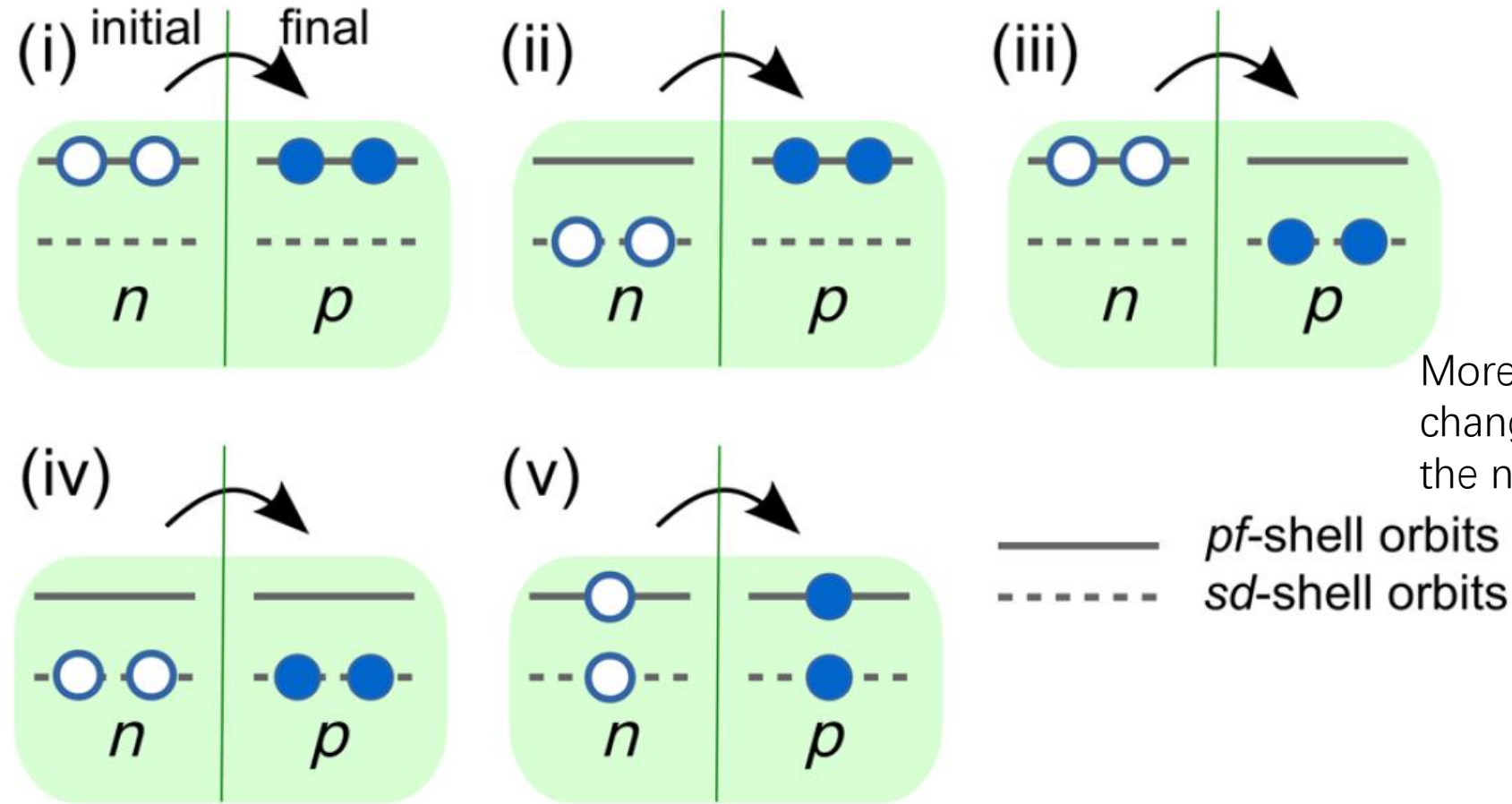


FIG. 3. NME decomposition in terms of the angular momentum and parity  $J^\pi$  of the pair of decaying neutrons, Eq. (3).  $0\hbar\omega$  (GXPF1B) and  $2\hbar\omega$  (SDPFMU-DB) results are compared, without short-range correlations.

**$^{48}\text{Ca}$ :** Y. Iwata, N. Shimizu, T. Otsuka, Y. Utsuno, J. Menéndez, M. Honma, and T. Abe, PRL 116, 112502 (2016).

# Choice of model space



More channels are open, which change the pairing structure, and the node structure..

**<sup>48</sup>Ca**: Y. Iwata, N. Shimizu, T. Otsuka, Y. Utsuno, J. Menéndez, M. Honma, and T. Abe, PRL 116, 112502 (2016).



## CCM SRC

F. Simkovic, A. Faessler, H. Muther, V. Rodin, and M. Stauf, Phys. Rev. **C79**, 055501 (2009)

CCM SRC is fitted to Correlated 2-bd wavefunction of CCM ( $S_2$  correlation) / H.O. 2-bd wavefunction in the relative Coordinate, in the  $S_0$  channel with node as 0 ( $R_{\{n=0,l=0\}}$ ).

To get rid off the node dependence of the correlated wavefunction? SRC will change if the other choices are made.

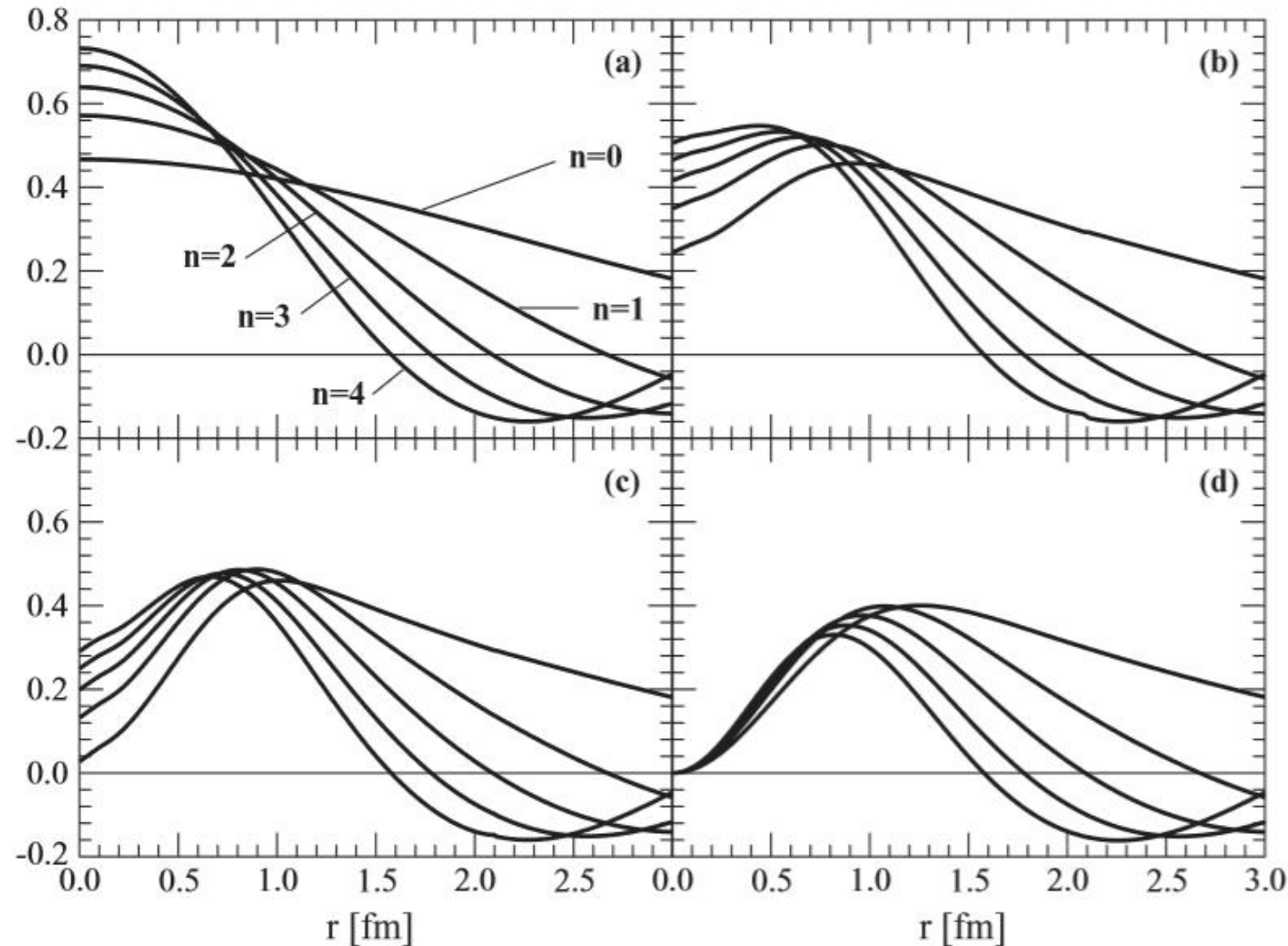


FIG. 1. Two-nucleon wave functions as a function of the relative distance for the  $^1S_0$  partial wave and radial quantum numbers  $n = 0, 1, 2, 3$ , and 4. The results are for the (a) uncorrelated two-nucleon wave functions, (b) coupled-cluster method with CD-Bonn potential, (c) coupled-cluster method with Argonne potential, and (d) Miller-Spencer Jastrow short-range correlations. The harmonic oscillator parameter  $b$  is 2.18 fm.

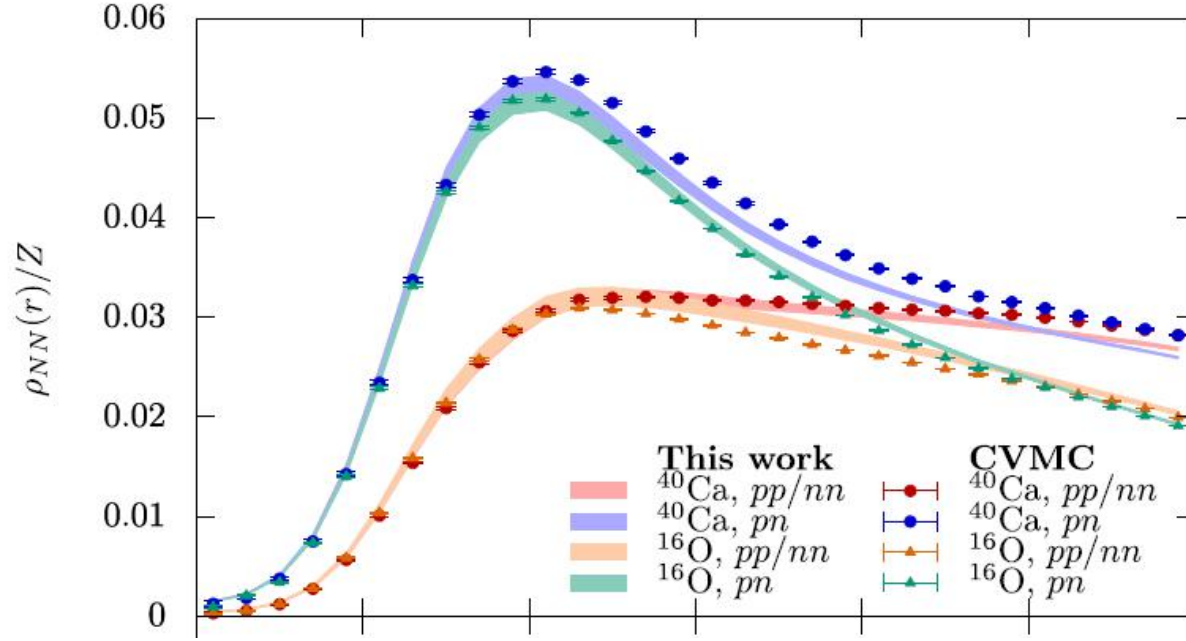
### Introduce a new parameter “c”:

It means that at  $r = 0$ , the 2-bd w.f. is not zero (not eliminated by the hard core).

## CCM SRC

- There is systematic difference between CCM SRC and traditional SRC (MS SRC):
  - ((1))CCM SRC's peak is at 1.0 fm, but MS SRC's peak is at 1.5 fm. So MS SRC will shift the peak of NME distribution toward 1.5 fm (NME w/o SRC peak at 1.0 fm), but CCM SRC does not shift NME distribution. So CCM SRC maintain the original peak position.
  - ((2))MS SRC eliminate the distribution at  $r=0$  completely (C parameter =0); CCM SRC does not.

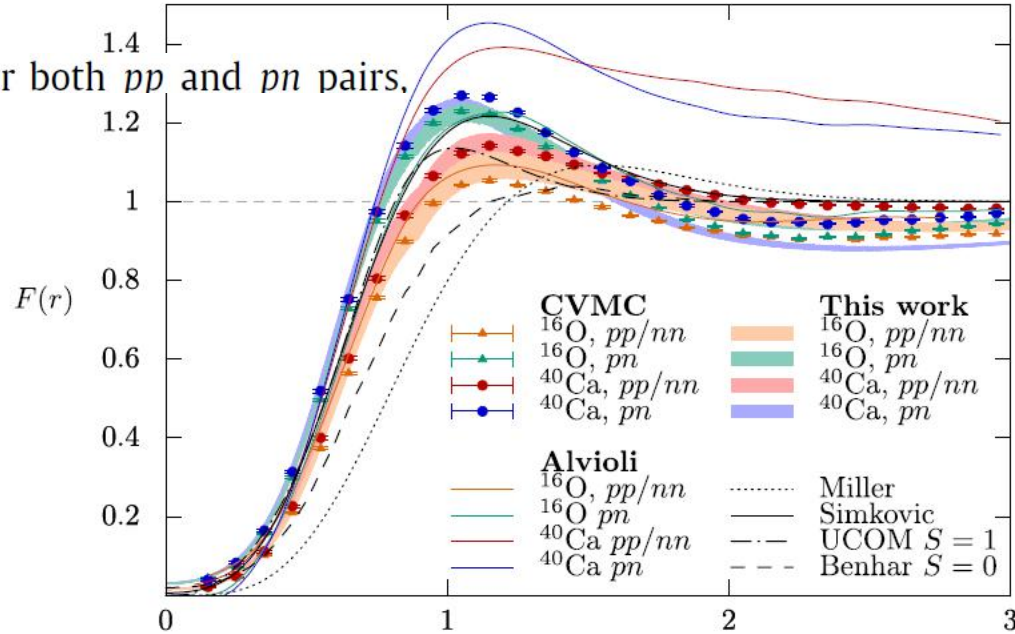
## CVMC SRC



For convenience, we provide the following parameterization for the  $pp/nn$  and  $pn$  correlation functions determined from CVMC:

$$F(r) = 1 - e^{-\alpha r^2} \times \left( \gamma + r \sum_{i=1}^3 \beta_i r^i \right) \quad (11)$$

correlation functions for both  $pp$  and  $pn$  pairs.



**Table 1**

Parameters describing  $F(r)$ , using the functional form of equation (11).

Parameter	Units	Value ( $pp/nn$ )	Value ( $pn$ )
$\alpha$	$\text{fm}^{-2}$	3.17	1.08
$\gamma$	–	0.995	0.985
$\beta_1$	$\text{fm}^{-2}$	1.81	–0.432
$\beta_2$	$\text{fm}^{-3}$	5.90	–3.30
$\beta_3$	$\text{fm}^{-4}$	–9.87	2.01