

 \mathbb{Z}^4 , \mathbb{Z}^2

Ab initio description of doubly open-shell nuclei via a novel multi-reference perturbation theory École Thématique PhyNuBe, Aussois, Aussois, Aussois, Aussois, Aussois, Aussois, Aussois, Aussois, Aussois, Aus

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[1] M. Frosini, T. Duguet, J.-P. Ebran, V. Somà, **arXiv:2110.15737**

[2] M. Frosini, T. Duguet, J.-P. Ebran, B. Bally, T. Mongelli, T.R. Rodríguez, R. Roth, V. Somà, **arXiv:2111.00797**

[3] M. Frosini, T. Duguet, J.-P. Ebran, B. Bally, H. Hergert, T.R. Rodríguez, R. Roth, J.M. Yao, V. Somà, **arXiv:2111.01461**

⦿ **Introduction**

⦿ **PGCM-PT formalism**

⦿ **PGCM results**

⦿ **PGCM-PT(2) results**

⦿ **Outlook**

Ab initio nuclear chart

Ab initio

Hamiltonian describes "bare" NN & NNN interactions

(Approximate) solution must be systematically improvable and approach the exact solution

Ab initio nuclear chart

⦿ **Further progress hindered by**

- Storage cost of Hamiltonian matrix elements (method-independent)
- Runtime & memory costs of many-body calculations (method-dependent)

➝ **Exponential scaling**

➝ **Mixed scaling**

➝ **Polynomial scaling**

Closed- vs open-shell nuclei $11C$ ϵ **21 ⁶⁸ Ni ⁷⁸ Ni 7/2 ^g 9/2 ⁴⁸ Ni ⁵⁶ Ni p 1/2 f 5/2 ^p 3/2 Zlosed- vs open-shell nuclei**

Single- vs multi-reference strategy

- **U(1)**-breaking
	- ➝ Gorkov SCGF, BMBPT, BCC
- **SU(2)**-breaking
- → Deformed CC
	- Symmetry restoration
		- \rightarrow Theory developed (excpet GF) [Duguet 2015]
		- \rightarrow Implementation: work in progress \rightarrow PGCM-PT
- IR physics via diagonalisation
	- → Multi-configuration PT
	- ➝ *Diagonalisation step impacts scalability*
- **○ This work: IR physics via PGCM**
	- → Exploits symmetry breaking + restoration
	- ➝ *Symmetry-conserving & low dimensional*
	-

Single- vs multi-reference strategy

⦿ Introduction

⦿ **PGCM-PT formalism**

⦿ **PGCM results**

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⦿ **Outlook**

Unperturbed state 3.1 PGCM unperturbed states 1.1 $\mathbf{1}$ PGCM unperturbed state 3.1 PGCM unperturbed states and the state of the state of
2.1 PGCM unperturbed state of the state of th as *q* 6= 0. Because physical states must carry good relations, which PGCM-PT o↵ers to do consistently. Because of the incorporation of static correlations into 3.1 PGCM unperturbed state

symmetry quantum numbers one acts on *|*(*q*)i with

typically defined such that the product states belonging

⦿ **Construction of the unperturbed state via projected generator coordinate method (PGCM)** ction of the unperturbed state via projected generator coordinate method (PGCM) symmetry group G*H*. See App. B for a discussion of the symmetry group G*H*. See App. B for a discussion of the symmetry group G*H*. See App. B for a discussion of the σ^2 $\left($ **PCCM** *Projected generator coordinate method (I GCIVI)* $\mathbf{a} = \mathbf{a}$ action of the unpertunced state via projected generator coo on of the unperturbed state via projected generator coordinate method (PGCM) $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$ $M^2(M)$ *R*(*R*(*R*) and *R*(*R*) and *R*(*R*) and R truction of the unperturbed stat *inate method (PCCM)* rotation operator *R*(*Q*) and the IRREP *D*

the operator of the operator

 μ uct states (\leftarrow EDF) es (\leftarrow EDF) **∂** Dwedimensional linear combination of *v* t <u>non-c</u> rthogonal Bogolyuboy product sta dimensional l duct states (+ EDF) ○ Low-dimensional linear combination of *non-orthogonal* Bogolyubov product states (← EDF)

☆ NOCI eigenvalue problem expressed in a set of non-orthogonal projected HFB states α states \mathcal{A} as a matrix state can be written as \mathcal{A} in a practical calculation.

Perturbative expansion 2.1 Set up *^µ ,* (9b) where \mathbf{X} ⇣ *^H*⁰ *^E*(0)⌘ right-hand-side of Eq. (13) iteratively and sort out the terms with expansion

The present work focuses on the perturbative expansion of the perturbative expansion of the perturbative expansi
The perturbative expansion of the perturbative expansion of the perturbative expansion of the perturbative ex

of the wave operator. Starting from Eqs. (5)-(6), the

The goal is to compute the goal is to compute the perturbative corrections to compute the perturbative correct
The perturbative corrections to compute the perturbative corrections to compute the perturbative corrections o

to first exact state and energy as $\frac{1}{\sqrt{2}}$, where $\frac{1}{\sqrt{2}}$, where $\frac{1}{\sqrt{2}}$

Q , (14a)

^h⇥(0)*|H*¹

expansion is defined using the so-called *intermediate*

Working algebraic expressions of *[|]*⇥(*k*)

^µ = 0 such that *^P*˜

ⁱ and *^E*(*k*) are

¹a *,* (23a)

¹Aa ⁼ ^a*†*H¯ ¹^a *,* (23b)

. . .

 $\overline{}$

\odot Formal perturbation theory *Q* ⌘ 1 *P* \odot Formal perturbation theory n theory

to7,8

spanning the latter eigen subspace of *H*⁰ are *not* assumed

 \blacksquare

where the superscript *k* indicates that the corresponding

 $\overline{}$

i*,* (10a)

, (10b)

- \circ Introduce partitioning $H = H_0 + H_1$ of the wave operator. Starting from Eqs. (5)-(6), the the partitioning $\boldsymbol{\Pi} = \boldsymbol{\Pi}_0 + \boldsymbol{\Pi}_1$ \circ Introduce partitioning $H = H_0 + H_1$ \sim introduced above are stated above are stated above are stated as \sim 1 \overline{a}
- \circ Expand exact wave function and energy as $\ket{\varPsi}\equiv\sum|\varTheta^{(k)}\rangle$ and $\frac{\infty}{\frac{1}{\cdot}}$ $k=0$ $|\Theta^{(k)}\rangle$ and $E \equiv \sum E^{(k)}$ $\frac{\infty}{\frac{1}{\cdot}}$ $k=0$ $\ket{\text{exact}}$ wave function and energy as $\ket{\Psi}\equiv\sum\ket{\Theta^{(k)}}$ and $E\equiv\sum E^{(k)}$ *we function and energy as* $|\Psi\rangle \equiv \sum_i |\Theta^{(k)}\rangle$ and $E \equiv \sum_i E^{(k)}$ -1 ${\bf H}$ ⁰ + ${\bf H}$ ¹ *K [|]*⇥˜*^K ^µ* ih⇥˜*^K ^µ | ,* (9a) $\overline{k=0}$ $k=0$ \mathbf{u} the degenerate states obtained via symmetry transfer \circ Expand exact wave function and energy as ∞ to the unperturbed ∞ $\equiv \sum_i |\Theta^{(\kappa)}\rangle$ and $E \equiv \sum E^{(\kappa)}$ $k=0$ and $k=0$ \circ l α and α α α α $\ket{\text{and exact wave function and energy as} \ket{\Psi} \equiv \sum_{k=0}^{N} |\Theta^{(k)}\rangle \text{, and}$

artitioni
^ ิ
เท: *ig* the Findert space via the projectors \circ Perturbative corrections can be identified by partitioning the Hilbert space via the projectors artitioning the Hilbert spa w=0
Martitioning the Hilbert space via the projectors parameters are indere by \circ Perturbative corrections can be identified by partitioning the Hilbert space via the projectors energy of the full Hamiltonian are written as *|* i and *E*, .

 $k \equiv 0$ Model space $\longleftarrow \qquad \mathcal{P} \equiv |\Theta^{(0)}\rangle\langle\Theta^{(0)}| \qquad \mathcal{Q} \equiv 1 - \mathcal{P} \qquad \longrightarrow \qquad \text{External space}$ quantity are proportional to the *k*th power of *H*1. This *^E*ref ⌘ h⇥(0)*|H|*⇥(0)ⁱ ⁼ *^E*(0) ⁺ *^E*(1) *.* (17) σ the complementary orthogonal subspace, the so-complementary order σ $Nioael space$ $P = |\Theta^{\vee} \rangle \langle \Theta^{\vee} |$ $r = 1 \quad \mathcal{D}$ is Extended sorts $\epsilon = 1$ μ μ ^{1.} μ ^{1.} Aodel

Q ⌘ 1 *P* are introduced. The operator *^P*˜ \circ Second-order energy correction reads spanning the latter eigen subspace of *H*⁰ are *not* assumed $t₁$ \circ H ₁ H ₁ H ² H ₁ H ₂ H ₂

and, as such, depend on the quantum numbers (*µ,* ˜),

where κ indicates the superscript κ indicates that the corresponding κ indicates the corresponding κ $\ket{\Theta^{(1)}} = -\mathcal{Q}\left(H_0 - E^{(0)}\right) \quad \mathcal{Q}H_1\ket{\Theta^{(0)}}$ (2) $\mathcal{L}(\mathbf{Q}(0)|\mathbf{H} \mathbf{Q}(\mathbf{Q}(1)))$ where $\mathcal{L}(\mathbf{Q}(1)) = \mathcal{L}(\mathbf{H} \mathbf{P}(\mathbf{Q}(0)))^{-1} \mathcal{L}(\mathbf{H} \mathbf{Q}(\mathbf{Q}(0)))$ $s^{(2)} = \langle \Theta^{(0)} | H_1 \mathcal{Q} | \Theta^{(1)} \rangle$ where $|\Theta^{(1)} \rangle = -\mathcal{Q} | \mathcal{Q} |$ *ZECON FCGGS*
(1) $\sqrt{(1)}$ $\sqrt{(1)}$ $\sqrt{(H - F(0))}^{-1}$ $\sqrt{(H - F(0))}$ The two series do not yet provide the perturbative cor- $\langle 1 \rangle$ where $|\Theta^{(1)} \rangle = -Q(H_0 - E^{(0)})$ QH_1 formations, i.e. belonging to the same irreducible repre- $\left. \begin{array}{c} \text{or} \quad \text{if} \quad$ $\Gamma(2)$ $\Gamma(0)$ III $\Omega(\Omega)$ is the state $\Gamma(0|1)$ $\Omega(T)$ *^H*⁰ ⁼ *^E*(0)*|*(0)ih(0)*[|]* ⁺ $\mathcal{O}[H_1]$ $x + 1$ *^E^I [|]^I* ih*^I [|]* $\begin{bmatrix} 0 & 1 \\ 0 & 1 \end{bmatrix}$ $|\Theta^{(1)}\rangle = -\mathcal{Q}$ $E^{(2)} = \langle \Theta^{(0)} | H_1 \mathcal{Q} | \Theta^{(1)} \rangle$ where $| \Theta^{(1)} \rangle = -\mathcal{Q} \left(H_0 - E^{(0)} \right)^{-1} \mathcal{Q} H_1 | \Theta^{(0)} \rangle$

eigenstates of H_0 are known, one can invert and obtain algebraic expressions $\qquad \qquad \Big\}$ $E^{(2)} = -\sum_{I} \frac{1}{I} \frac{1}{E^{I} - E^{(0)}}$ *,* **8***k* **1** *x* **1** S_{R} $\mathcal{H} = E^{(0)} |\varPhi^{(0)}\rangle\langle\varPhi^{(0)}| + \sum_{i=1}^{N} E^{I} |\varPhi^{I}\rangle\langle\varPhi^{I}| \quad \longrightarrow \quad E^{(2)}$ $\begin{array}{ccccc} \overline{a} & \over$ called *Q* space. In the present context, the eigenstates $S.D_{\perp/\pm}(0)$ $\left| \frac{1}{\pi} \frac{1}{\pi} I_1 \right|^2$ $\sum_{i=1}^{\infty} |\langle \varPhi^{(0)} | H_1 | \varPhi^I \rangle|$ $\sum_{I} \frac{E^I - E^{(0)}}{E^I - E^{(0)}}$ $\frac{1}{\sqrt{13}}$ is the contract out the Eq. (13) iteratively and solution of Eq. (13) iteratively and solution out the contract out out th $\sum_{S,D}$ $\sum_{i=1}^{N,D,\ldots} \frac{\mathcal{O}(D)}{\mathcal{O}(D)} |H_1|$ $\begin{array}{ccccc} \tau & \swarrow & \rightarrow & \rightarrow & \rightarrow & \rightarrow & \rightarrow & \tau & \tau & \tau & \tau \end{array}$ spanning the latter eigen subspace of *H*⁰ are *not* assumed presence of *^E ^E*(0) on the right-hand side through *^Y* . \mathcal{L} is necessarily contribution, it is necessarily contribution, it is necessarily contributed by \mathcal{L} $\left| \begin{matrix} 2 & \\ & \end{matrix} \right|$ right-hand-side of Eq. (13) iteratively and sort out the terms with equal powers of *H*1. This procedure leads If eigenstates of *H0* are known, one can invert and obtain algebraic expressions *^E*ref ⌘ h⇥(0)*|H|*⇥(0)ⁱ ⁼ *^E*(0) ⁺ *^E*(1) *.* (17) $H_0 = E^{(0)} |\Phi^{(0)}\rangle\langle\Phi^{(0)}| +$ *S,D,...* \sum *I* $E^I |\Phi^I\rangle \langle \Phi^I |$ *^E*(2) ⁼ ^h⇥(0)*|H*1*A|*⇥(0)ⁱ ⁼ ^h*† ^E*(3) ⁼ ^h⇥(0)*|H*1*A*²*|*⇥(0)ⁱ ⁼ ^h*†* $E^{(2)} = -\sum$ *I S,D I* $\left|\langle\varPhi^{(0)}|H_{1}|\varPhi^{I}\rangle\right|$ $\overline{\mathsf{I}}$ 2 $E^{I} - E^{(0)}$ $\begin{bmatrix} 1 & 1 \end{bmatrix}$ if eigenstates of H_0 are known, one can i the notations. Consequently, the targeted eigenstate and the targeted eigenstate and $S_{1}D_{2}...$ $H_0 = E^{(0)} |\Phi^{(0)}\rangle\langle\Phi^{(0)}| + \sum_{\alpha} E^{\alpha} |\Phi^{\alpha}\rangle\langle\Phi^{\beta}|$ Γ and unperturbed state and energy state and ene *[|]*⇥(1)ⁱ ⁼ *X*¹*QH*1*|*⇥(0)i*,* (15b) ⁼ h⇥(0)*|H*1*QX*¹*QH*1*|*⇥(0)i*,* (16b) $\frac{S.D + (I^2 O)(I^2 - I^2)}{2}$. .. and
9 an Dùbhlach
9 an Dùbhlach μ eigenstates of μ_0 are Ki $\langle E^{(0)}|\Phi^{(0)}\rangle\langle\Phi^{(0)}|\nonumber +\sum_{l=1}^{\infty}\langle E^{l}|\Phi^{l}\rangle\langle\Phi^{l}|\nonumber -\sum_{l=1}^{\infty}\langle E^{l}|\Phi^{l}\rangle\langle\Phi^{l}|\nonumber -\sum_{l=1}^{\infty}\langle E^{l}|\Phi^{l}\rangle\langle\Phi^{l}|\nonumber -\sum_{l=1}^{\infty}\langle E^{l}|\Phi^{l}\rangle\langle\Phi^{l}|\nonumber -\sum_{l=1}^{\infty}\langle E^{l}|\Phi^{l}\rangle\langle\Phi^{l}|\nonumber -\sum_{l=1}^{\infty}\langle E^{l}|\Phi^{l}\rangle$ ⁼ ^h⇥(1)*|QH*¯1*Q|*⇥(1)i*,* (16c)

one eigen ^h⇥(0)*[|]* ⁱ = 1 *.* (12) spanning the latter eigen subspace of *H*⁰ are *not* assumed μ -orthogonal FT (present case). Only one eigenstate of μ_0 is Known μ_0 term^s with extensive powers of *H₁* to be known explicitly. Non-orthogonal PT (present case): only one eigenstate of *H0* is known prthogonal PT *S PT* (present case): $\ddot{\cdot}$ 2 knowing that *E*(1) = (*H*1)00. are denoted as *[|]*⇥(0)ⁱ and *^E*(0) to typify that they act **EXECUTE:** Non-orthogonal PT (present case): only one eigenstate of H_0 is known . . .

with the degenerate states obtained via symmetry trans-

- *n* well-defined Hilbert-space partitioning, projector Q cannot be explicitly constructed \vert $\mathcal{L}(\mathcal{$ → No well-defined Hilbert-space partitioning, projector *Q* cannot be explicitly constructed *[|]*⇥(1)ⁱ ⁼ *X*¹*QH*1*|*⇥(0)i*,* (15a) *[|]*⇥(2)ⁱ = +*X*¹*QH*¯1*QX*¹*QH*1*|*⇥(0)i*,* (15b) $\overline{}$ No well defined Hilbert enece partition *E* No well-defined Hilbert-space partitioning, projector Q cannot be ex-
- *a* $\left\{\n \begin{array}{ccc}\n \text{MOCI-PT} & \text{[Burton & Thom 2020]} \\
 \text{[Burton & Thom 2020]} & \text{[Buroth]} \\
 \text{[Barton & Theorem 2020]} & \text{[Buroth]} \\
 \text{[Barton & Theorem 2020]} & \text{[Buroth]} \\
 \text{[Brain & Theorem 2020]} & \text{[Buroth]} \\
 \text{[Brain & Theorem 2020]} & \text{[Buroth]} \\
 \text{[Brain & Theorem 2020]} & \text{[Buroth$ → Rigorous PT formalised only recently: NOCI-PT [Burton & Thom 2020] *[|]*⇥(2)ⁱ = +*X*¹*QH*¯1*QX*¹*QH*1*|*⇥(0)i*,* (15b) the notations. Consequently, the targeted eigenstate and $\overline{}$ Rigorous PT formalised only recently: N 8The perturbative expansion of the wave operator formally stated the wave operator for the wave operator formally stated the wave operator for the wave operator for the wave operator for the wave operator for the wave oper

those labels are dropped for the time being the time being the time being the time being to light experimental
The time being to light the time being the time be

Perturbative expansion \mathbf{L} wave function is given by ϵ and any of the overlap with any of the overlap with any of the other HFBB ϵ vacua making up *[|]*⇥(0)i, and thus with *[|]*⇥(0)ⁱ itself. Even-*Perturbative expansion* t critativative expandioni Perturbative expansion unperturbed states to a single (unconstrained) and \mathbf{u} r critativative expansio angle of the orientation of the orientation of the orientation of the orientation of $\mathbf P$ tribute to *E*(2) if it corresponds to a linear combination $\overline{}$ Γ outurle otizzo. Otro era bet of the parties of Expansion *^E*(2) ⁼h⇥(0)*|*(*^H ^E*ref)*|*⇥(1)ⁱ (55)

vacuum h(p_{rin}g), _in double excitations. E2⁰ to its double excitations. E20 to its double exc

\circ Non-orthogonal perturbation theory \odot Non-orthogonal perturbation theory \odot Non-orthogonal perturbation theory $\hfill B$

separable form

cientification and contact the contact of the contact of

Baranger 1-body Hamiltonian
tonian H₂ $T_{\rm eff}$ that, as pointed out in Sec. 3.2.3, the first-order out in Sec. 3.2.3, the first-order order this goal, one interaction-state-specific partition-specific partition-specific partition-space space space sp
Support the space s uniquely contributing to *E*(2), it is thus sucient to first-order interactions of \overline{p} and \overline{p} an Baranger 1-body Hamiltonian
<u>N</u> ^h(*p*; ✓)*|*(*HE*ref)*|^I* (*p*; ✓)ih*^I* (*p*; ✓)*|*⇥(1)ⁱ \mathcal{O} the excitation rank is naturally truncated given \mathcal{O}

{a^I (*q*); *^q* ² set and *^I* ² S,D,T,. . . *} .*

X

denote the unknowns to be determined.

*I*2*S,D*

tually, this means that (i) *Q* cannot be built explicitly

f ⇤

sibly different representation at players \mathcal{L} at players \mathcal{L} at players \mathcal{L} at players \mathcal{L} at players \mathcal{L}

M0(✓)

µ(*p*)*D*˜

edly, the second one requires a procedure to optimally

non-orthogonal states

system, *F*[*|*⇥i] would be nothing else but the so-called Baranger

non-orthogonal states

 α

 $\mathcal{L}_{\mathcal{A}}$

we called $\epsilon = \epsilon \approx \epsilon, \epsilon, \epsilon$

 μ , where $T \in \mathcal{D}, \mathcal{D}, \mathcal{I}, \dots$

which is unmanageable in practical applications. The problems of the practical applications. The problems of the

influenced by the presence of higher-rank excitations in the presence of higher-rank excitations in the presence

^a^I (*q*)*|*⌦*^I* (*q*)i*,* (52)

is either in *Q* or *P* space. In expanded form, the linear

approximation given that, even if only single and double

⁰⁰*|*⇥¯(1)ⁱ (50)

^Q^A ⁼ *QH*¯¹ *,* (19)

*^E*ref ⌘ h⇥(0)*|H|*⇥(0)ⁱ ⁼ *^E*(0) ⁺ *^E*(1) *.* (17)

of single and double excitations associated with a (pos-

[|]⇥(1)i ⌘ *^P* ˜

=

Hartree-Fock (HF) Slater determinant 17. Slater determinant 17. Slater determinant 17. Slater determinant 17.
To achieve determinant 17. Slater determinant 17. Slater determinant 17. Slater determinant 17. Slater determi

d˜

- \circ Construct reference Hamiltonian H_0 to H_0 if $\overline{H_2}$ if $\overline{H_3}$ if $\overline{H_4}$ is a linear combination of $\overline{H_3}$ if $\overline{H_4}$ is a linear combination of $\overline{H_3}$ is a linear combination of $\overline{H_4}$ is a linear combination of $\overline{H_5}$ is a \circ Construct reference framification r_{10}
	- \to Introduce state-specific partitioning $H_0\equiv \mathcal{P}^{\tilde{\sigma}}_\mu F_{[|\Theta\rangle]}\mathcal{P}^{\tilde{\sigma}}_\mu+\mathcal{Q}^{\tilde{\sigma}}_\mu F_{[|\Theta\rangle]}\mathcal{Q}^{\tilde{\sigma}}_\mu$ orthogonal component to *[|]*⇥(0)i, Eq. (51) is used to $\mathbb{E}_{[\Theta \rangle]} \mathcal{P}^{\tilde{\sigma}}_{\mu} + \mathcal{Q}^{\tilde{\sigma}}_{\mu} F_{[|\Theta \rangle]} \mathcal{Q}^{\tilde{\sigma}}_{\mu}$ c partitioning $H_0 \equiv \mathcal{P}_\mu^\sigma F_{|{\Theta} \rangle} \mathcal{P}_\mu^\sigma + \mathcal{Q}_\mu^\sigma F_{|{\Theta} \rangle} \mathcal{Q}_\mu^\sigma$ sibly) di↵erent representation at play. Looking for the $\mathbb{V}[\ket{\Theta}] \mathcal{Q}_{\mu}$ \to Introduce state-specific partitioning $H_0 \equiv \mathcal{P}_\mu^{\tilde{\sigma}} F_{[[\Theta \rangle]} \mathcal{P}_\mu^{\tilde{\sigma}} + \mathcal{Q}_\mu^{\tilde{\sigma}} F_{[[\Theta \rangle]} \mathcal{Q}_\mu^{\tilde{\sigma}}$ σ , μ which drastically reduces the cardinality of the set of duce state-sp Γ Ω ^{$\tilde{\sigma}$} \mathfrak{C}^{\prime} $\left| \ket{\theta} \right|$ \mathcal{Z}_{μ} \rightarrow Inti $\tilde{\sigma}$ and $\tilde{\sigma}$ $\tilde{\sigma}$ $[\psi_{\mu} + \mathcal{Q}_{\mu}^{\dagger} F_{\lbrack} | \Theta \rangle] \mathcal{Q}_{\mu}^{\dagger}$ denote the unknowns to be determined.
The unknowns to be determined to be determined to be determined to be determined. $\begin{array}{ccccc} \text{I} & \text{I} & \text{I} & \text{I} & \text{I} & \text{II} & \text$ $\tilde{\sigma}$ $\bar{\sigma}$ where the excitation rank is naturally truncated given \mathcal{L} $\mathcal{L}_{\mu}I^{\prime}||\theta\rangle|\mathcal{L}_{\mu}$

One-body operator $F(\rho(\Theta))$ *such that Møller-Plesset partitioning is recovered in the single-determinant limit* Rather than referring to the orthonormal representation ming is recovered in the single-determinant limit *[|]*⇥(1)ⁱ ⁼ ^X X *^a^I* (*q*)*|*⌦*^I* (*q*)i*,* (52) fully fixes the dependence of these coecients on the ng is recovered in the single-determinant limit One-body operator $F(\rho(\Theta))$ such that Møller-Plesset partitioning is recovered in the single-dete uniquely contribution to the extension of the *E*(2), it is the *E*(2), it is thus such that σ in the single-determinant limit where the one-body operator \mathbf{t} One-body operator $F(\rho(\Theta))$ such that Møller-Plesset partitioning is recovered in the single-determinant limit *[|]*⇥(1)ⁱ ⁼ ^X vacuum h(*p*; ✓)*|* to its double excitations. E↵ectively, ered in the single-determinant limit

○ Construct first-order wave function Explicitly projecting onto *Q* space to only retain the orthogonal wave function

Component to *a* \circ Construct first-order wave function $\frac{1}{2}$ and $\frac{1}{2}$ *Post-order wave function*

 $\mathbf v$

 $\overline{}$ schematically in Fig. 3, the fig. 3, the

 $\overline{}$

[|]⇥(1)ⁱ ⁼ ^X

 \rightarrow Build all possible excitations on top of each Bogolyubov state entering $\ket{\Theta^{(0)}}$, then $\frac{1}{2}$ $\frac{1}{2}$ ations on top of each Bogolyubov state entering $\ket{\Theta^{(0)}}$, then ations on top of each Bogolyubov state entering $\ket{\Theta^{(0)}}$, then $\overline{\text{ing}} \mid \Theta$ d all possible excitations on top of each Bogolyubov state entering $\ket{\Theta^{\rm (0)}}$, then *3.3.3 Equation of motion* orthogonal component to *a* contract to *a*[{] α [}] α [}] α [}] α [}] α [}] α *}* α [}] α *}* \rightarrow Build all possible excitations on to Ruild all possible excitations on top of each Bocolumboy $\frac{1}{2}$ of the order parameters on the order $\frac{1}{2}$ order $\frac{1}{2}$ order $\frac{1}{2}$ \circ contourned $|O(0)|$ then e entering $|\Theta^{(0)}\rangle$, then te entering $|\Theta^{(0)}\rangle$ then σ interacting space spanned by product states σ

 $\mathcal{L} = \mathcal{L} \mathcal{L}_{00} | \mathcal{L}_{(q)} \rangle$ orthogonal component to *[|]*⇥(0)i, Eq. (51) is used to Excited Bogolyubov vacua, where $I \in S$, D , T ,... $\begin{array}{cc} \begin{array}{ccc} \nearrow & \end{array} & \begin{array}{ccc} \nearrow & \end{array} & \begin{array}{ccc} \nearrow & \end{array} \end{array}$ $\langle \Omega^I(q) \rangle \equiv \mathcal{Q} P^{\sigma}_{00} | \Phi^I(q) \rangle$ *[|]*⇥(*k*)ⁱ with *k >* 1. $\frac{1}{2}$ standard matrix rely on an unperturbed matrix $\frac{1}{2}$ on an unperturbed matrix relation to an unperturbed matrix relation to an unperturbed matrix relations of the stress of the stress relations of the stress iyubov vacua, where $I \in \mathcal{S}, \mathcal{D}, \mathcal{I}, \dots$ $| \Omega^I (q) \rangle \equiv \mathcal{Q} P^{\tilde{\sigma}}_{0 0} | \varPhi^I (q) \rangle$ $\overline{I} \subset S \cap T$ Excited Bogolyubov vacua, where $I \in S, D, T, \ldots$ $\frac{Q}{q} \sum_{I} (1)^{1-\epsilon} (1)^{I}$ where $\frac{P}{q} (1)^{I}$ $|(q)|\Omega^{T}(q)\rangle$ \mathbb{R}^2 *I* (*d*)^{*i*} \equiv $QP_{00}^{\circ}|\Phi^{\prime}(q)\rangle$ by definition \overline{I} involves the convolution of the two-body interaction $\det B$ *south a symmetry-independent above* $I \in S$ D.T. $|\Theta^{(1)}\rangle = \sum \sum a^{I}(q)|\Omega^{I}(q)\rangle$ where *q* \sum *I* $a^I(q)|\Omega^I(q)\rangle$ where $|\Omega^I(q)|$ $\emph{Excited Bogolyubov vacu}$ $\frac{1}{\sqrt{2}}$ U_{here} $I \in S \cap T$ by vacua, where $I \in S$,D,T,... $\vert \epsilon$ $\langle \mathcal{P}^{(1)} \rangle = \sum_{q} \sum_{I} a^{T}(q) | \mathcal{Q}^{T}(q) \rangle$ where $\overline{J}(x, y) = \overline{J}(x, y)$ The last step of the process consists in determining the $\ket{\Theta^{(1)}} = \sum$ *a*_{*I*} *1* (*q*) *1* (*x*) *a*_{*I*} (*x*) *n* (*x*) *1* (*x* $\mathcal{O} = \mathcal{O}D\tilde{\sigma} |\mathcal{A}|_{\mathcal{L}}$ $\mathcal{S} = 2 \cdot 100 \frac{V}{\epsilon}$ (9). first-order interacting space spanned by product states $\langle \Phi \rangle \equiv \mathcal{Q} P_{\rm oo}^{\tilde{\sigma}} |\Phi^{I}(q)\rangle$ include single and double excitations from each Bogoli- ν a where $I \in S.D.T...$

 $|\varTheta^{(1)}\rangle$ ated partitioning have been introduced, the perturbative \circ Compute second-order energy as a function of $=H$ - H_0 and $\ket{\Theta^{(1)}}$ *a* Compute second-order $3.33 \times 10^{(1)}$ \circ Compute second-order energy as a function of $H_1 = H$ - H_0 and $\vert \Theta^{(1)} \rangle$ $\left(1 \right)$ $i\in(1)$ $|\Theta_{\langle\tau\rangle}\rangle$

wave-function is thus expanded over \mathcal{C} is thus expanded over $(0,1)$

Explicitly projecting onto *Q* space to only retain the

In principal and \overline{S} , and \overline{S} are involved in Eq. (53), and \overline{S} , and \overline{S} , and \overline{S} , and \overline{S}

^a^I (*q*)*|*⌦*^I* (*q*)i*,* (52)

l \overline{q} $\overline{I} \in S, D$ θ Oply $|\phi^{I}(q)|$ with $I \subset S$ D contribute ϵ defining the PGCM-PTC ϵ and ϵ partitioned [12] as it is built out of single and double excitation of single and double excitaoproximate $\langle \Theta^{(1)} \rangle = \sum_{n=1}^{\infty} a^I(q) | \Omega^I(q) \rangle$ $\frac{p}{q}$ $\frac{p}{f \in S.D}$ norm *q* of the order parameter. \overline{q} $\overline{I} \in S, D$ \overline{N} \overline{N} \overline{L} \overline{L} \rightarrow Only $|\Phi'(q)\rangle$ with $I \in S$, D contribute \rightarrow Approximate $|\Theta^{(1)}\rangle = \sum_{\alpha} \sum_{q} a'(q) | \Omega'(q) \rangle$ *[|]*⇥(1)ⁱ ⁼ ^X \overline{CD} step of the process consistence of the process consistent \overline{CD} and \overline{CD} an $\sum_{q} A_{q}$ contribute \rightarrow Approximate $\sum_{q} A_{q}$. the matrix A of *A* is the solution of the system of linear $\rangle = \sum$ MA ⁼ H¯ ¹ *,* (20) $I_0(1)$ $\sum_{i=1}^{\infty} I_{(i)}(0)$ te -> Approxima $q \quad I \in S,D$ $\frac{1}{2}$ $\frac{1}{2}$ A s schematically illustrated in \mathcal{A} schematically in \mathcal{A} , the fig. 3, the fi $q = \sum$ q. 1 \in S,D. \rightarrow Only $|\Phi^{I}(q)\rangle$ with $I \in S, D$ contribute \rightarrow Ap *q J*2*S,D* $\langle A^{I}(q)|\Omega^{I}(q)\rangle$ *Only* $|\Phi^{I}(q)\rangle$ with $I \in S$,D *contril* $|\Theta^{(1)}\rangle = \sum_{}^{} \sum_{}^{}~ a^{I}(q)|\Omega^{I}(q)\rangle$ |
|
|
| S, D *^a^I* (*q*)*|*⌦*^I* (*q*)i*.* (56) *q* $\sum \; \, a^{I}(q)|\varOmega^{I}(q)\rangle$ *I*2*S,D*

where $\mathbf{M} \equiv \mathbf{H}_0 - E^{(0)}\mathbf{1}$ $\overline{}$ schematically in Fig. 3, the ideal is to the expansion of \mathbf{r} that the fact that $\mathbf{r}(0)$ $\mathbf{v}(\mathbf{r})$ where $\mathbf{v}(\mathbf{r}) = \mathbf{v}(\mathbf{r})$ tion to *[|]*⇥(1)ⁱ delivers a variational upper bound to *^E*(2) *q I* We be the expansion $\sum_{q} \sum_{J \in S, D} \frac{M I_p J_q u}{y} (q) = -n_1(p)$ where $M = H_0 - E^{(0)} I$ \sum *q* \sum *J*2*S,D* $M_{IpJq} a^{J}(q) = -h_1^{I}(p)$ where $\mathbf{M} \equiv \mathbf{H}_0 - E^{(0)} \mathbf{1}$ necessarily belongs to *Q* space whereas the right index where $J(\lambda)$ is the energy-independent independent independent independent independent independent independent independent independent in $J(\lambda)$ $p q a (q) = -h_1(p)$ where $M \equiv H_0 - E^{(0)} I$ $\sum_{i} \sum_{j} \mathbf{V}_{j} \math$ μ of the order equation $\sum_{x \in \mathcal{C}} \sum_{p}$ excitations contribute to the contributions are $\mathbf{M} = \mathbf{H}_o = E^{(0)} \mathbf{1}$ influenced by the presence of higher-rank excitations in the wave function \mathcal{P} and the linear system \mathcal{P} $\sum M_{\tau} = \alpha^{J}(\alpha) \sum_{a} \sum_{l \in S} \sum_{l} e^{i2} h^{l} q^{l}$ norm *q* of the order parameter. with \overline{I} 2 \overline{I} 2 \overline{I} 2 \overline{I} 2 \overline{I} 2 \overline{I} 3 \overline{I} (p) where $M \equiv H_0 - E^{(0)} 1$ excitations contribute to the energy contribute to the energy contribute to the coecients are coecients are co $\sum_{M_{\tau}} M_{\tau} = a^{J}(q) - b^{I}(p)$ **rewrite Solution** $\sum_{\alpha} \sum_{\alpha} M I p J q u$ Master equation

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⦿ **PGCM-PT(2) results**

⦿ **Outlook**

1. Constrained HFB Mey ₇₆ 2.0 -78 20 Ne [HFB] 1.6 -80 -82 1.2 -84 β_3 -86 0.8 -88 -90 0.4 -92 -94 0.0 $-0.30.0$ 0.3 0.6 0.9 1.2 1.5 β_2

20Ne

⦿ **Constrained HFB calculations** lowest-energy path, with the arrow positioned at the \bullet Constrained HFB calculations

- Maps total energy surface (TES) \mathbf{M} states used in the subsequent \mathbf{C} (FFC). \circ Maps total energy surface (TES)
- Minimum at strongly deformed configuration Ω ^{1.}88 Ω
- \circ TES soft along the octupole direction

the axial (2*,* 3) plane. The (red) full line indicates the

20Ne

N³LO EFT Hamiltonian with srg = 1*.*88 fm¹.

charge radius is 0*.*02 fm (0*.*7%).

2⁺ states are 830 keV (0*.*7%) and 810 keV (0*.*7%), respectrum in the uncertainty of uncertainty on the uncertainty of uncertainty on the ground-state ground-state

Furthermore, the impact of *e*3max has been studied by varying the truncation parameter in the range *e*3max =

8 14 for selected observables. Overall, both energies

⦿ **Projected HFB calculations** lowest-energy path, with the arrow positioned at the \bullet Projected HFB calculations \bullet 2⁺ states are 830 keV (0*.*7%) and 810 keV (0*.*7%), re-

○ Projections favour deformed configurations $\mathbf{F} \cdot \mathbf{F}$ states used in the subsequent PGCM calculation. \circ Projections favour deformed configurat σ deformed configurations charge radius is 0*.*02 fm (0*.*7%).

N³LO EFT Hamiltonian with srg = 1*.*88 fm¹.

varying the truncation parameter in the range *e*3max =

8 14 for selected observables. Overall, both energies

the axial (2*,* 3) plane. The (red) full line indicates the

- Negative parity states accessed srg = 1*.*88 fm¹.
- o Provide input for computing PGCM state and \vert

20Ne

⦿ **PGCM mixing** \overline{a} arrow path, with the arrow position position position \overline{a} \bullet PGCM mixing dots characterize the set of the set of

 \circ Collective w.f. \rightarrow admixture of PHFB states \overline{C} H_c \overline{C} H_c \overline{C} states used in the subsequent PGCM calculation. \circ Collective w.f. \rightarrow admixture of PHFB s spectively, whereas the uncertainty on the ground-state charge radius is 0*.*02 fm (0*.*7%).

N³LO EFT Hamiltonian with srg = 1*.*88 fm¹.

the axial (2*,* 3) plane. The (red) full line indicates the

- Significant shape fluctuations srg = 1*.*88 fm¹.
- o Negative parities mix more deformations and all as \vert

20Ne

\odot PGCM excitation spectrum

○ Reference: in-medium no-core shell model (IM-NCSM) [Mongelli & Roth] nR oforonco: in modium no care shall modal (IM NCSM) IMongolli & Rothl

- → Good agreement with experiment and (quasi-)exact IM-NCSM (in e2fm4) are indicated along vertical arrows whereas a selection of *E*3 transition strengths (in e3fm6) are indicated
- → Essential static correlations captured by PGCM
- freedom. Panel (b): PHFB results based on the HFB configuration configuration corresponding to the minimum of the $\frac{1}{2}$ \rightarrow Exaggerated collectivity [B(E2) systematically larger than experiment]
- \rightarrow Bostricting PCCM to 1D or PHFR deteriorates spectrum modeling i SCM to 1D of THE deteriorates specifianties. ➝ Restricting PGCM to 1D or PHFB **deteriorates spectrum**

Neon chain λ istot λ

o Dynamical correlations essential for I \circ PT+projection provide good indication $\begin{array}{cccc} 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 \end{array}$ Ω R ¹ and *corrected* by P C M \overline{a} B_{max} is the state dependent of the experimental ground-state \sim rms charge radius along the Neon isotopic charge r ○ PT+projection provide good indication **Formula** corrected by PGCM Hamiltonian with srg = 1*.*88 fm¹ is employed in mical correlations essentian EVAL portant and in 24 Ne, radii associated with the HFB minisymmetry-conserving scheme, i.e. on top of the PGCM dii: trend corrected by PGCM already be appreciated through through the results of single-symmetric of single-symmetric of single-symmetric \circ Dynamical correlations essential for B.E. $\frac{1}{\sqrt{2}}$ ○ Radii: trend corrected by PGCM

- 2. Solution is experienced orbital associated with the last of Eestius Correlation energies (up-tated with the l
1. The Eestius Correlation energies (up-tated with the last of Eestius Correlation energies of the last of Ee and the shell is indicated with a shell simulation of the shells is indicated with a black dotted with a black σ \circ Good description dittle \sim 1 σ ○ Good description until 24Ne
- \circ 30 Ne off the trend ¹⁸32Ne. First *E*²⁺ ¹ and *E*⁴⁺ \circ ³⁰Ne off the trend $P(X|X) = P(X|X)$ ○ ³⁰Ne off the trend
- ^o Heavier isotopes too collective in PC Baranger's spherical shell structure [60,61] along the $P = 2000$ results with model-space (black box) plus $P = 2000$ plus EFTE \circ Heavier isotopes too collective in PGCM T most important feature for the present discussion of the pres $\boldsymbol{\mathsf{M}}$ is challenging. Several methods exist to $\boldsymbol{\mathsf{M}}$ ○ Heavier isotopes too collective in PGCM N3LO EFT Hamiltonian with srg = 1*.*88 fm¹ is em-

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⦿ **PGCM-PT(2) results**

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PGCM-PT(2) validation

⦿ **First proof-of-principle calculation in a small model space (emax=4)**

- NN interaction only
- Compare to exact Full CI reference [R. Roth]

⦿ **Doubly closed-shell 16O**

- Radius as collective coordinate
- GCM yields small effect in closed-shells
- GCM-PT(2) gets close to FCI
- MBPT(2,3) consistent at canonical point

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- Quadrupole def. as collective coordinate
- Projection brings 5 MeV binding
- PGCM-PT(2) brings in dyn. correlations
- \circ dMBPT(2,3) underbinds \rightarrow projection needed

PGCM-PT(2) validation

12
12 March 12 March 1
12 March 12 March 1

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- PGCM-PT(2) brings in dyn. correlations
- \circ dMBPT(2,3) underbinds \rightarrow projection needed
- PGCM-PT(2) preserves quality of exc. spectra

Combining PGCM-PT(2) with MR-IMSGR *S*GR **H**₁

 α M its elementary α exclude dependents s multi-telefone mond. Hackers acpendent \bullet Multi-reference IMSRG: nucleus-dependent transformation of H $H(s) = U^{\dagger}(s)HU(s)$

 \circ Decouples $|\Theta^{(0)}\rangle$ from Q space as $s \to \infty$ \longrightarrow Dynamical correlations recast into H(s)

of *H*^A associated with a preferred reference vacuum

I

E^I E(0)

 \circ PGCM+MR-IMSRG recently explored by Yao et al. \rightarrow Promising results; impact of PT? γ Tromising results, impact

- \rightarrow Problem becomes more perturbative Prostem secomes more perturbative
- → PT(2) correction systematically decreases

- \rightarrow Problem becomes more perturbative \rightarrow PT(2) corrects for dilatation of spectrum \mathbf{B} $PT(2)$ cors
	- → Triaxial GCM not enough

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Towards the ab initio description of complex nuclei

⦿ Three complementary levers to tackle complex mid-mass/heavy nuclei via expansion methods

1. Pre-processing of the Hamiltonian

 \rightarrow Flow must resum bulk of dynamical correlations without inducing a large break of unitarity

2. Choice of reference state

- \rightarrow Rich enough to capture non-perturbative static correlations, but low dimensionality
- **3. Systematic expansion of the many-body Schrödinger equation**
	- \rightarrow Low-order truncation with gentle scaling

Optimal balance between the three must be found

⦿ **Novel multi-reference perturbation theory**

- PGCM accounts for collective/IR correlations
- UV physics provided by well-defined non-orthogonal PT
- Can be combined with pre-processing of *H*

