# Ab initio Calculation of Nuclear Matrix Elements of Neutrinoless Double Beta Decay with the IMSRG+GCM approach

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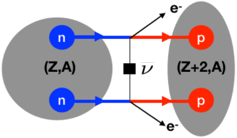
# Nuclear matrix element for neutrinoless double beta decay

- The NME for the $0\nu\beta\beta$ transition from $|0_i^+\rangle$ to $|0_f^+\rangle$

$$M^{0\nu}(0_i^+ \to 0_f^+) = \langle 0_f^+ | O^{0\nu} | 0_i^+ \rangle$$




  – the transition operator: exchange of light neutrinos and with closure approximation

$$O^{0\nu} = \frac{4\pi R}{g_A^2} \int d^3\vec{x}_1 \int d^3\vec{x}_2 \int \frac{\int d^3\vec{q}}{(2\pi)^3} \frac{e^{i\vec{q}\cdot(\vec{x}_1-\vec{x}_2)}}{q[q+\bar{E}-(E_i+E_f)/2]} \mathcal{J}_\mu^\dagger(\vec{x}_1)\mathcal{J}^{\mu\dagger}(\vec{x}_2)$$

  – the effective nuclear current

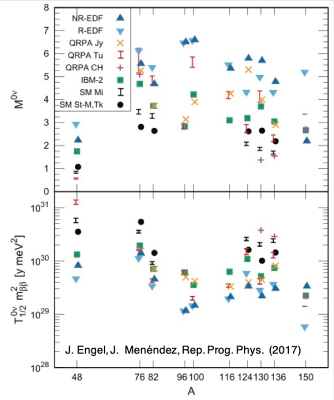
$$\mathcal{J}_\mu^\dagger(x) = \bar{\psi}(x)\left[g_V(q^2)\gamma_\mu - g_A(q^2)\gamma_\mu\gamma_5 + i g_M(q^2)\frac{\sigma_{\mu\nu}}{2m_p}q^\nu - g_P(q^2)q_\mu\gamma_5\right]\tau^+\psi(x).$$

# Nuclear matrix element for neutrinoless double beta decay

– the transition operator in non-relativistic reduction form

$$O^{0\nu} = \frac{2R}{\pi g_A^2}\int_0^\infty q\,dq \sum_{a,b} \frac{j_0(qr_{ab})[h_F(q)+h_{\rm GT}(q)\vec{\sigma}_a\cdot\vec{\sigma}_b] + j_2(qr_{ab})h_T(q)[3\vec{\sigma}_j\cdot\hat{r}_{ab}\vec{\sigma}_k\cdot\hat{r}_{ab}-\vec{\sigma}_a\cdot\vec{\sigma}_b]}{q+\bar{E}-(E_i+E_f)/2}\tau_a^+\tau_b^+$$

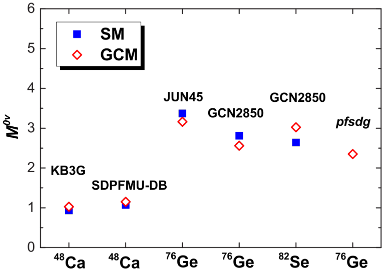
$$\begin{aligned}
h_{F\text{-VV}}(q^2) &= -g_V^2(q^2),\\
h_{\text{GT-AA}}(q^2) &= -g_A^2(q^2),\\
h_{\text{GT-AP}}(q^2) &= \frac{2}{3}g_A(q^2)g_P(q^2)\frac{q^2}{2m_p},\\
h_{\text{GT-PP}}(q^2) &= -\frac{1}{3}g_P^2(q^2)\frac{q^4}{4m_p^2},\\
h_{\text{GT-MM}}(q^2) &= -\frac{2}{3}g_M^2(q^2)\frac{q^2}{4m_p^2},\\
h_{T\text{-AP}}(q^2) &= h_{\text{GT-AP}}(q^2),\\
h_{T\text{-PP}}(q^2) &= h_{\text{GT-PP}}(q^2),\\
h_{T\text{-MM}}(q^2) &= -\frac{1}{2}h_{\text{GT-MM}}(q^2).
\end{aligned}$$



# Nuclear matrix element for neutrinoless double beta decay

## Source of discrepancy among different models

- Different effective interactions
- Many-body methods with different level of approximations




Jiao, Engel, Holt (2017)

- For a given (effective) Hamiltonian, shell model and GCM predict similar values for the NME.

# ab initio methods for neutrinoless double beta decay

## Ab initio methods in the sense that

- starts from a bare nucleon-nucleon interaction (fitted to *NN* scattering data)
- solves Schroedinger equation (for the many-body system) with a controllable accuracy of approximations

– Benchmark calculations for light nuclei:

√ Variational Monte Carlo calculation starting from the Argonne v18 two-nucleon potential and Illinois-7 three-nucleon interaction for light nuclei S. Pastore et al. (2017)

√ No-core shell model calculations starting from chiral NN+3N interactions for light nuclei P. Gysbers et al., R. A. Basili et al.

– Extension to medium-mass candidate nuclei:

√ Application of coupled-cluster (S. Novario, G. Hagen, T. Papenbrock et al.) and valence-space in-medium similarity renormalization group (IMSRG) (C. Payne, R. Stroberg, J. Holt et al.) method starting from chiral NN+3N interactions for $0\nu\beta\beta$-candidate nuclei

√ Merging the multi-reference IMSRG with generator coordinate method (GCM) starting from chiral NN+3N interactions for $0\nu\beta\beta$-candidate nuclei
JMY, B. Bally, J. Engel, R. Wirth, T. R. Rodríguez, H. Hergert, arXiv:1908.05424

# The IMSRG+GCM method: procedure

**GCM**
define reference state

↓

**IMSRG**
evolve operators

↓

**GCM**
extract observables

- Wave function of the reference state (0+)

$$|\Phi^{JNZ}_{\rm ref}\rangle = \sum_Q F^{JNZ}_Q \hat{P}^J \hat{P}^N \hat{P}^Z |\Phi_Q\rangle$$

- Many-body density matrices

$$\rho^{pqr\cdots}_{stu\cdots} = \langle \Phi_{\rm ref} | A^{pqr\cdots}_{stu\cdots} | \Phi_{\rm ref} \rangle.$$

- Normal-ordered operators

$$H = E^{(0b)}(\lambda) + f_0^{(1b)}(\lambda) + \Gamma^{(2b)}(\lambda) + W^{(3b)}(\lambda) + \cdots$$

in terms of irreducible densities

$$\begin{aligned}
\lambda^p_q &= \rho^p_q, \\
\lambda^{pq}_{rs} &= \rho^{pq}_{rs} - \mathcal{A}(\lambda^p_r \lambda^q_s), \\
\lambda^{pqr\cdots}_{stu\cdots} &= \rho^{pqr\cdots}_{stu\cdots} - \mathcal{A}(\lambda^p_s \lambda^{qr\cdots}_{tu\cdots}) - \cdots - \mathcal{A}(\lambda^p_s \lambda^q_t \lambda^r_u \cdots)
\end{aligned}$$

**GCM**
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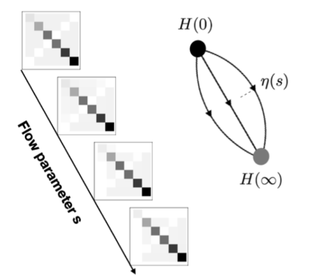
- Flow equation: $\frac{dH(s)}{ds} = [\eta(s), H(s)]$

where the $\eta(s) = \frac{dU(s)}{ds} U^\dagger(s)$ is the so-called generator chosen to decouple a given reference state from its excitations.




Tsukiyama, Bogner, and Schwenk (2011)
Hergert, Bogner, Morris, Schwenk, Tsukiyama (2016)

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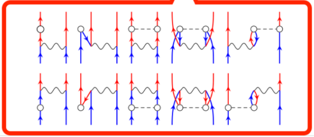
- Magnus: $U(s) = e^{\Omega(s)}$ $$\frac{d\Omega(s)}{ds} = \sum_{n=0}^{\infty} \frac{B_n}{n!} \mathrm{ad}^k_{\Omega(s)}(\eta(s))$$

  T. Morris (2015)

- Evolved NLDBD operators:

**$0\nu\beta\beta$ transition operator in IMSRG(2)**

$$O^{0\nu}(s) \equiv e^{\Omega(s)} O^{0\nu} e^{-\Omega(s)} = O^{0\nu} + [\Omega, O^{0\nu}] + \frac{1}{2}[\Omega, [\Omega, O^{0\nu}]] + \dots$$



# The IMSRG+GCM method: procedure

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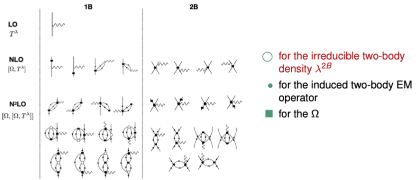
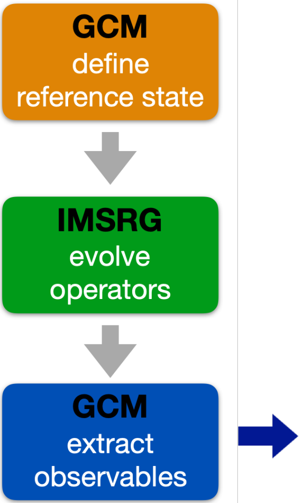
  T. Morris (2015)

- Evolved E2 operators:

$$T^{\lambda}(s) \equiv e^{\Omega(s)} T^{\lambda} e^{-\Omega(s)} = T^{\lambda} + [\Omega, T^{\lambda}] + \frac{1}{2}[\Omega, [\Omega, T^{\lambda}]] + \dots$$




Single-reference case: see *N. M. Parzuchowski et al. (2017)*




- Wave function of low-lying states

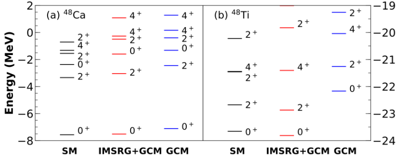
$$|\Psi^{JMZN}\rangle = \sum_{Q_i} F^{JZN}(Q_i)\,|JMZN(\mathbf{Q}_i)\rangle$$

- Hill-Wheeler-Griffin equation

$$\sum_{\mathbf{Q}_j}\left[\mathcal{H}^{JNZ}(\mathbf{Q}_i,\mathbf{Q}_j) - E^J\mathcal{N}^{JNZ}(\mathbf{Q}_i,\mathbf{Q}_j)\right]F^{JNZ}(\mathbf{Q}_j) = 0$$

where the kernels of operators $\hat{O}$ are defined as

$$O^{JNZ}(\mathbf{Q}_i,\mathbf{Q}_j) = \langle JNZ(\mathbf{Q}_i)|\hat{O}|JNZ(\mathbf{Q}_j)\rangle.$$




JMY, J. Engel, L. J. Wang, C. F. Jiao, and H. Hergert (2018)

# Applications

- Starting from a chiral NN(N$^3$LO) +3N (N$^2$LO) interaction (evolved with the free-space SRG) K. Hebeler et al. (2011)
- Benchmark calculations for light nuclei: $^{8}$He $\rightarrow$ $^{8}$Be and $^{22}$O $\rightarrow$ $^{22}$Ne
- Application to candidate $0\nu\beta\beta$ process: $^{48}$Ca $\rightarrow$ $^{48}$Ti

# Benchmark calculation: $0\nu\beta\beta$ from $^8$He to $^8$Be

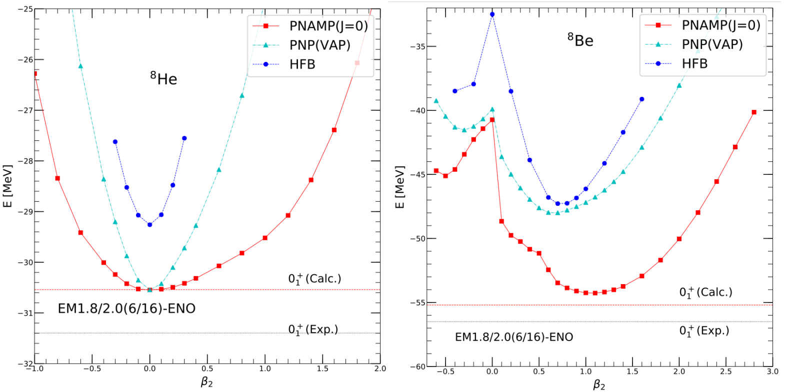
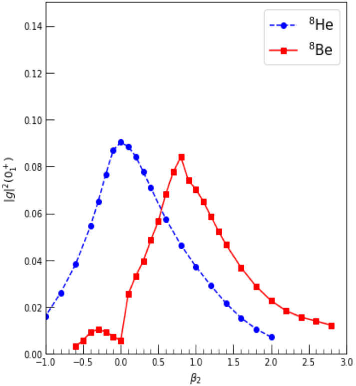
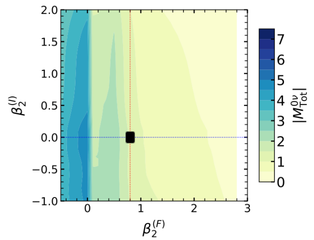
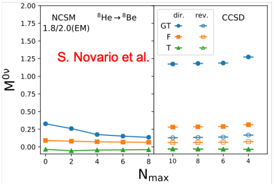



Figure: The potential energy surfaces from different calculations with $e_{\mathrm{Max}} = 6$, $\hbar\Omega = 16$ MeV.

# Benchmark calculation: $0\nu\beta\beta$ from $^8$He to $^8$Be




- IMSRG+PNAMP(Minimum): $M^{0\nu}_{\rm Tot}({\rm GT/F/TE}) = 1.40(1.19/0.28/-0.07)$
- IMSRG+GCM: $M^{0\nu}_{\rm Tot}({\rm GT/F/TE}) = 0.17(0.19/0.04/-0.06)$

# Benchmark calculation: $0\nu\beta\beta$ from $^{22}$O to $^{22}$Ne

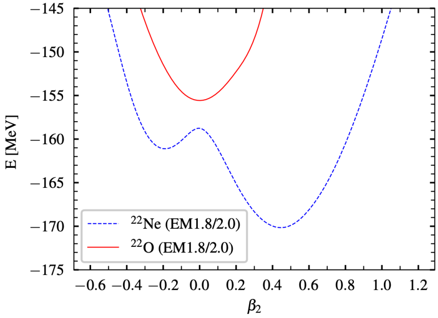
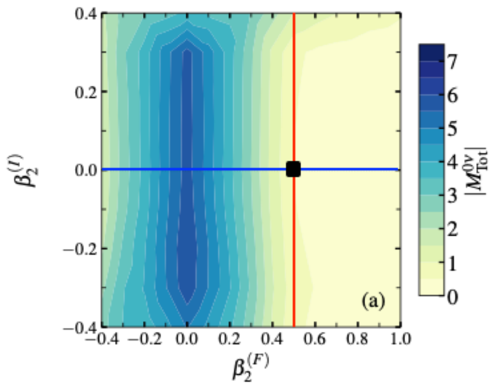
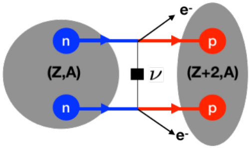


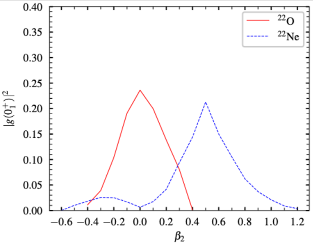

Figure: The potential energy surface from PNP (VAP)+HFB calculation with $e_{\rm Max} = 6$, $\hbar\Omega = 16$ MeV.

- $^{22}$O is dominated by spherical state
- $^{22}$Ne is dominated by prolate deformed state

# Application: $0\nu\beta\beta$ from $^{22}$O to $^{22}$Ne

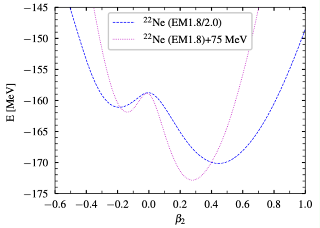


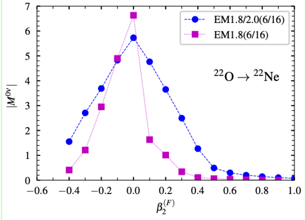



# Benchmark calculation: $0\nu\beta\beta$ from $^{22}$O to $^{22}$Ne

## Impact of the 3N interaction



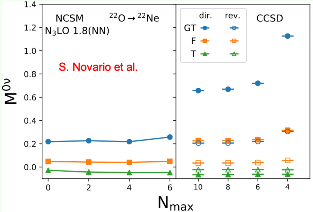

## IMSRG+PNAMP (minimum)

- $M^{0\nu} = 0.49$ by the 2N+3N interaction
- $M^{0\nu} = 0.34$ by the 2N interaction

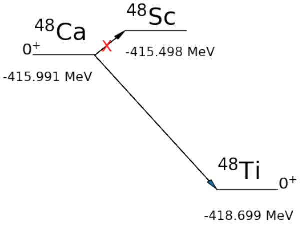
## IMSRG+GCM

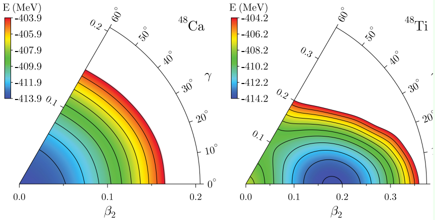
- $M^{0\nu} = 0.43$ by the 2N+3N interaction
- $M^{0\nu} = 0.15$ by the 2N interaction

## Results from NCSM and CC calcualtions



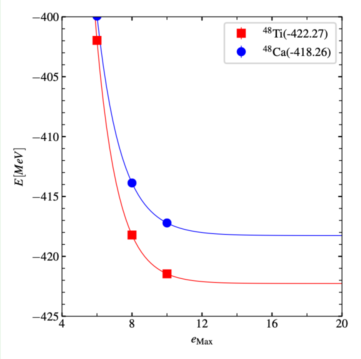
# Application: $0\nu\beta\beta$ from $^{48}$Ca to $^{48}$Ti



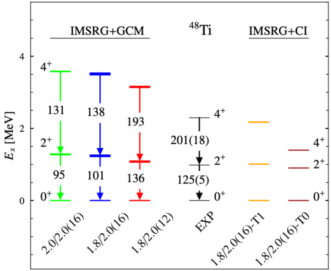




## Extrapolation

$$E(e_{\mathrm{Max}}) = E(\infty) + a\exp(-b \cdot e_{\mathrm{Max}})$$

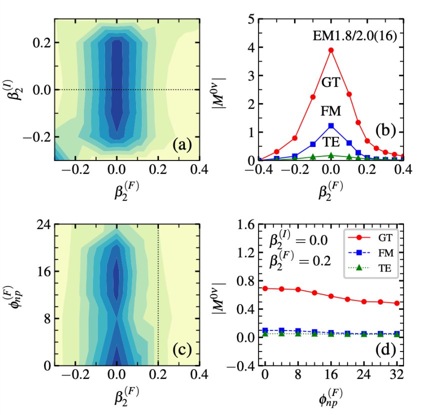


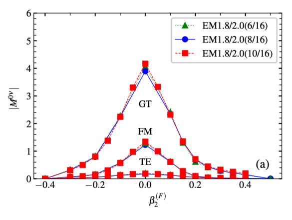
# Application: $0\nu\beta\beta$ from $^{48}$Ca to $^{48}$Ti

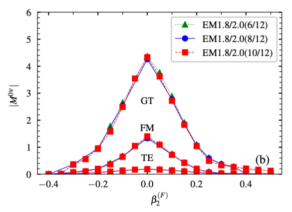



- IMSRG+GCM: Low-energy structure of $^{48}$Ti is reasonably reproduced (spectrum stretched). Inclusion of non-collective configurations from neutron-proton isoscalar pairing fluctuation can compress the spectra further by about 6%.
- IMSRG+CI(T0 $\rightarrow$ T1): the spectrum becomes more stretched in a larger model space (more collective correlations).

# Application: $0\nu\beta\beta$ from $^{48}$Ca to $^{48}$Ti



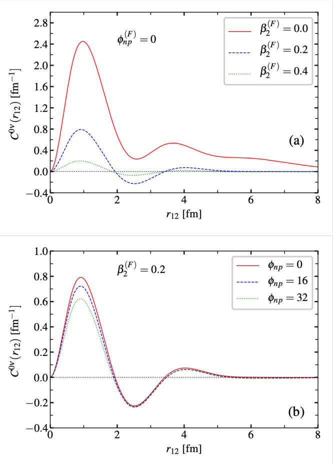




## Configuration-dependent NME

The $M^{0\nu}$ is decreasing dramatically with the quadrupole deformation, but moderately with $\phi_{np}$ at $\beta_2 = 0.2$ in $^{48}$Ti.

# Application: $0\nu\beta\beta$ from $^{48}$Ca to $^{48}$Ti



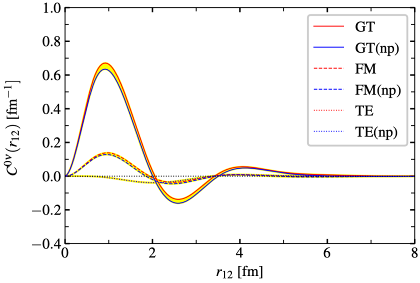

$$M^{0\nu} = \int dr_{12}\, C^{0\nu}(r_{12})$$

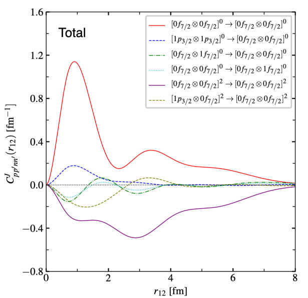
- The quadrupole deformation in $^{48}$Ti changes both the short and long-range behaviors
- Neutron-proton isoscalar pairing is mainly a short-range effect

$$C^{0\nu}(r_{12}) = \sum_{p\leq p', n\leq n'} \cdot \sum_J C^J_{pp'\,nn'}(r_{12}),$$

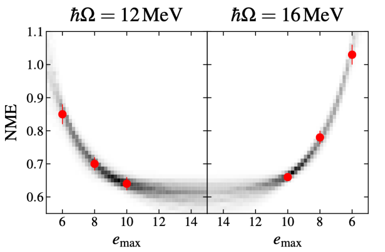
with

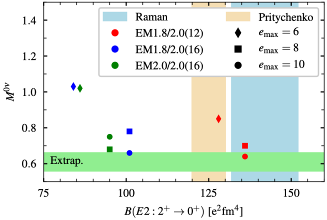
$$C^J_{pp'\,nn'}(r_{12}) = \frac{(2J+1)}{\sqrt{(1+\delta_{pp'})(1+\delta_{nn'})}} \langle (pp')J|\bar{O}^{0\nu}(r_{12})|(nn')J\rangle \rho^J_{pp'\,nn'},$$

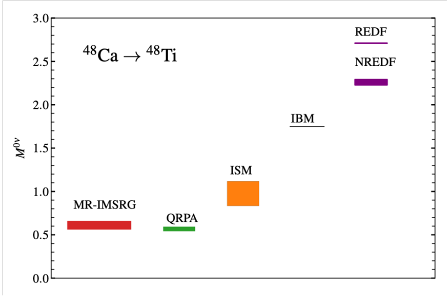


# Application: $0\nu\beta\beta$ from $^{48}$Ca to $^{48}$Ti (preliminary results)




- The value from Markov-chain Monte-Carlo extrapolation is $M^{0\nu} = 0.61^{+0.05}_{-0.04}$
- The neutron-proton isoscalar pairing fluctuation quenches $\sim$17% further, which might be canceled out partially by the isovector pairing fluctuation.

# Summary

Take-away messages:

- Worldwide ton-scale experiments are proposed to measure the $0\nu\beta\beta$ from which the determination of neutrino mass relies on the NMEs.
- Several groups have begun programs to calculate the NMEs from first principles, taking advantage of a flowering of ab initio nuclear-structure theory in the last couple of decades.
- The multi-reference IMSRG+GCM opens a door to modeling deformed nuclei with realistic nuclear forces (from chiral EFT). Many interesting phenomena of low-energy physics (shape transition, coexistence, cluster structure) can be explored within this framework.
- The NME from $^{48}$Ca $\rightarrow$ $^{48}$Ti is calculated from *first principles*.

What's next:

- Extension to heavier candidate nuclei, like $^{76}$Ge $\rightarrow$ $^{76}$Se and $^{136}$Xe $\rightarrow$ $^{136}$Ba.
- More benchmarks among several different *ab initio* methods for the NMEs.
- Quantification of uncertainties from different sources, impacts of induced three-body operators, two-body currents, contact transition-operator term, etc

# Collaborators and acknowledgement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**Iowa State University**

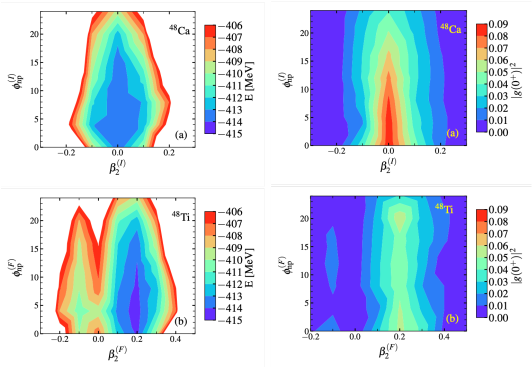
- Robert A. Basili
- James P. Vary

**Southwest University**

- Longjun Wang


Thank your for your attention!

# Application: $0\nu\beta\beta$ from $^{48}$Ca to $^{48}$Ti




- The *np* isoscalar pairing amplitude:

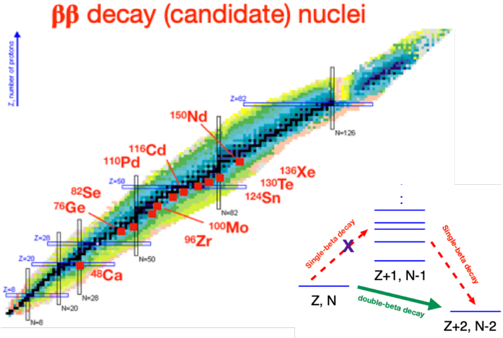
$$\phi_{np} = \langle \Phi | P_0^\dagger | \Phi \rangle + \langle \Phi | P_0 | \Phi \rangle$$

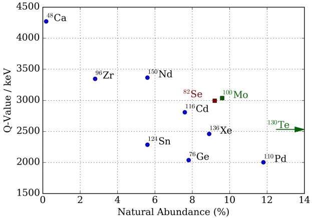
with

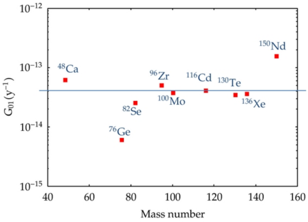
$$P_\mu^\dagger = \frac{1}{\sqrt{2}} \sum_\ell \hat{\ell} [a_\ell^\dagger a_\ell^\dagger]_{0\mu 0}^{L=0, J=1, T=0}$$

- Collective wave functions of g.s. extended along the $\phi_{np}$.

# Neutrinoless double beta-decay: contribution from nuclear physics




$$[T^{0\nu}_{1/2}]^{-1} = G_{0\nu} \left| \frac{\langle m_{\beta\beta} \rangle}{m_e} \right|^2 \left| M^{0\nu} \right|^2$$

where the phase-space factor $G_{0\nu}(\sim 10^{-14}\mathrm{yr}^{-1})$ can be evaluated precisely Kotila ('12), Stoica ('13). The effective neutrino mass is related to the masses $m_k$ and mixing matrix elements $U_{ek}$ of neutrino species