New GCM approach for $0\nu\beta\beta$

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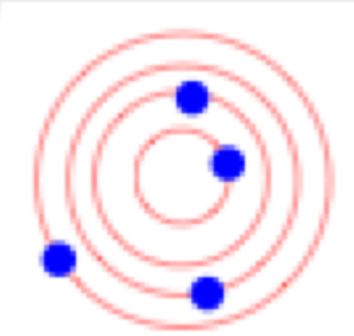
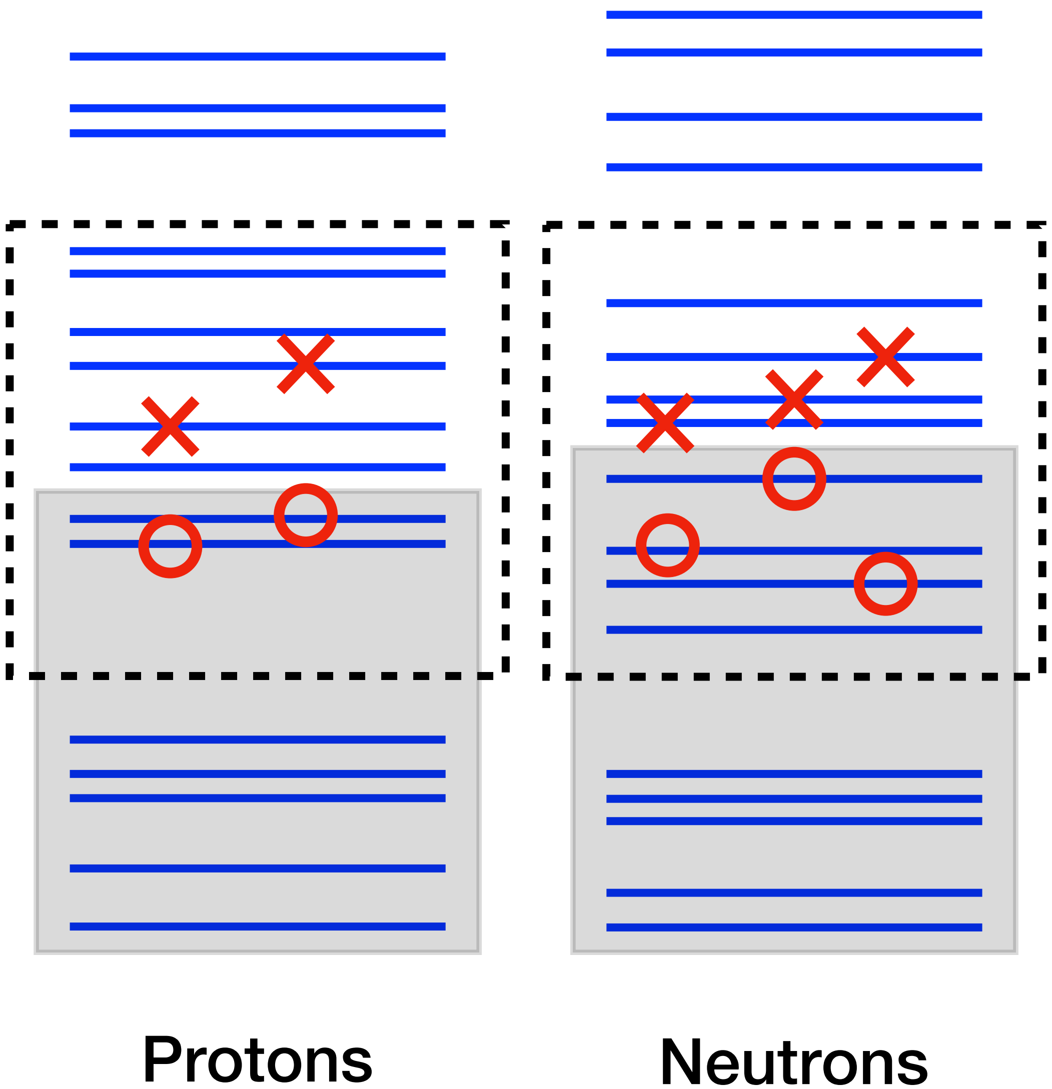
arXiv:1908.01873

Review of different Nuclear Models

Some models are built on single independent-particle state.





Shell model (SM)

$|0\rangle$

- Instead of solving Schrödinger equation in complete Hilbert space, one restricts the dynamics in a configuration space.

$$H|\Phi_i\rangle = E_i|\Phi_i\rangle \rightarrow H_{\rm eff}|\bar{\Phi}_i\rangle = E_i|\bar{\Phi}_i\rangle$$

Configuration interaction of orthonormal Slater determinants:

$$|\bar{\Phi}_i\rangle = \sum_j c_{ij}|\psi_j\rangle, \quad \langle\psi_j|\psi_k\rangle = \delta_{jk}$$

Diagonalizing the $H_{\rm eff}$ in the orthonormal basis.

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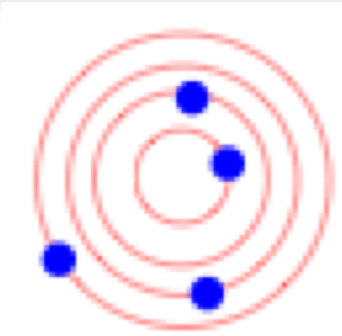
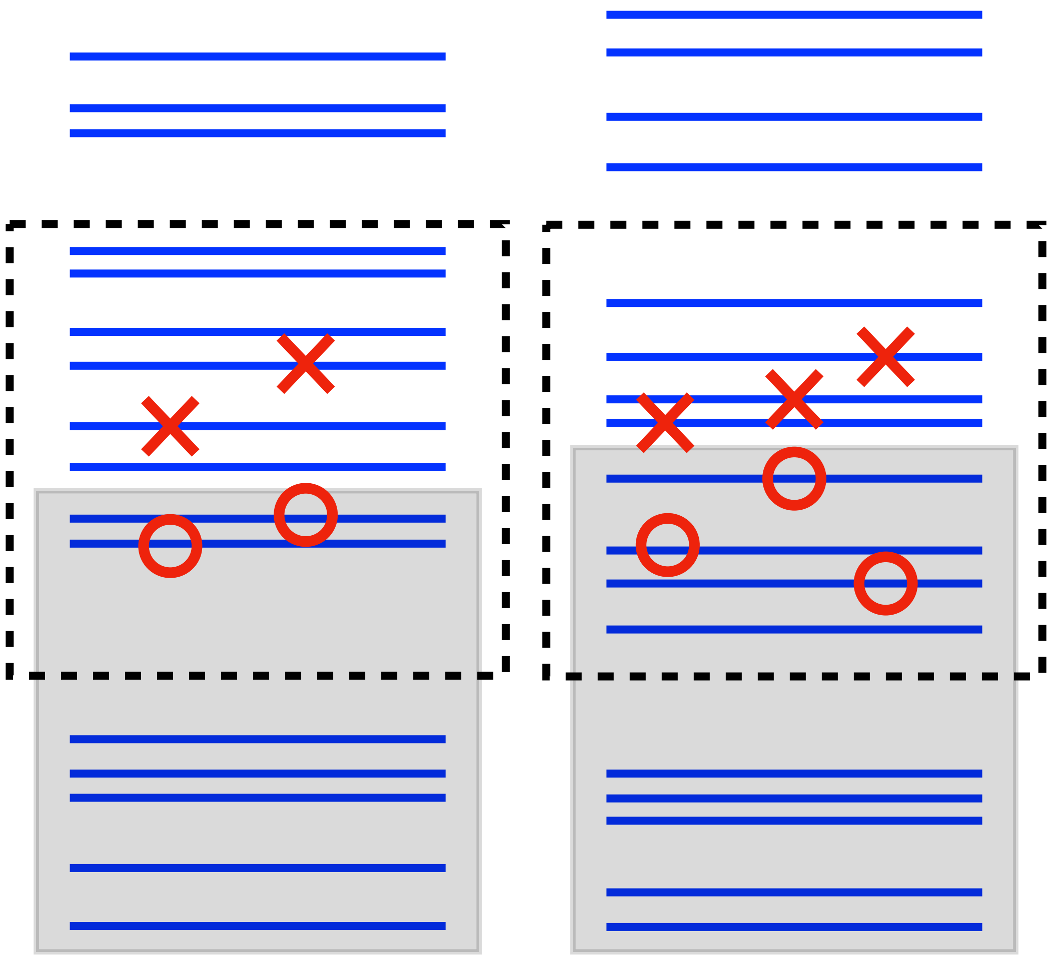




Shell model (SM)

Pros:

- Arbitrarily complex correlations within the model space.

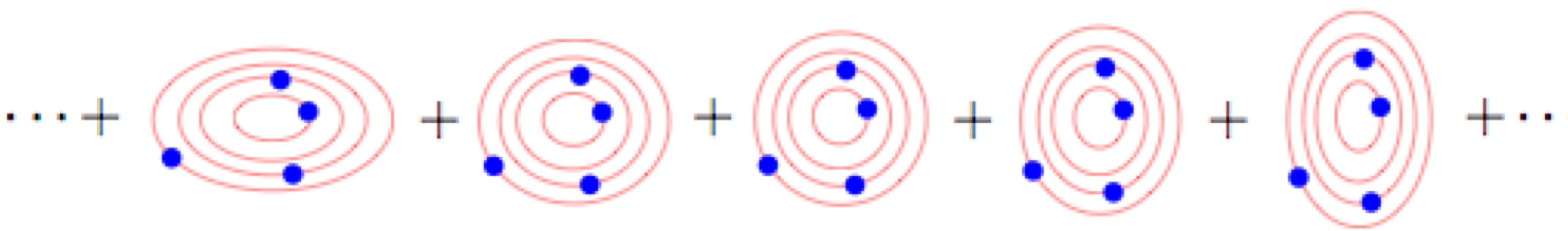
Cons:

- Relatively small configuration spaces.
  - at present the $0\nu\beta\beta$ decay NME calculations carried out by SM limited to one major shell.

The Other Way Around…

Another way to build many-body states:

Instead of configuration interaction with orthogonal states, one can diagonalize the Hamiltonian in a set of ***non-orthogonal*** basis.



$$|\Phi\rangle = \sum_j c_j |\psi_j\rangle, H_{jk} = \langle j|H|k\rangle$$

$$\sum_k H_{jk} c_k = E \sum_k N_{jk} c_k, N_{jk} = \langle j|k\rangle$$

The non-orthogonal states can be highly optimized, and hence reduce the dimension of basis states.

→ ***Generator-coordinate method***

Generator Coordinate Method

Generator Coordinate Method (GCM): an approach that treats large-amplitude fluctuations, which is essential for nuclei that cannot be approximated by a single mean field.

How it works:

① Step1: Construct basis states by constrained HFB calculation. correlations along important coordinates (e.g., deformation).

② Step2: Restore the symmetry of mean-field states. ***Projections.***

③ Step3: Diagonalize Hamiltonian in space of symmetry-restored nonorthogonal vacua.

GCM based on EDF has been applied to double-beta decay, however…

Generator Coordinate Method

Our long-term goal is to combine the virtues of both frameworks through an EDF-based or ab-initio GCM that includes all the important
shell model correlations and a large single-particle space.

Current achievement is the first step in this direction: CFJ developed a Hamiltonian-based GCM code in one and two (and possibly more) shells.

- More correlations.
- Larger model space.
- MPI parallelized for high performance computing.

How to Proceed?

- Using a realistic effective Hamiltonian.
- HFB states $|\Phi(q)\rangle$ with multipole constraints .

We "guess' the important collective correlations.

$$\mathcal{O}_1 = Q_{20}, \quad \mathcal{O}_2 = Q_{22},$$

$$\mathcal{O}_3 = \frac{1}{2}(P_0 + P_0^\dagger), \quad \mathcal{O}_4 = \frac{1}{2}(S_0 + S_0^\dagger),$$ *(isoscalar, isovector pairing)*

- Angular momentum and particle number projection

$$|JMK;NZ;q\rangle = \hat{P}^J_{MK}\hat{P^N}\hat{P^Z}|\Phi(q)\rangle$$

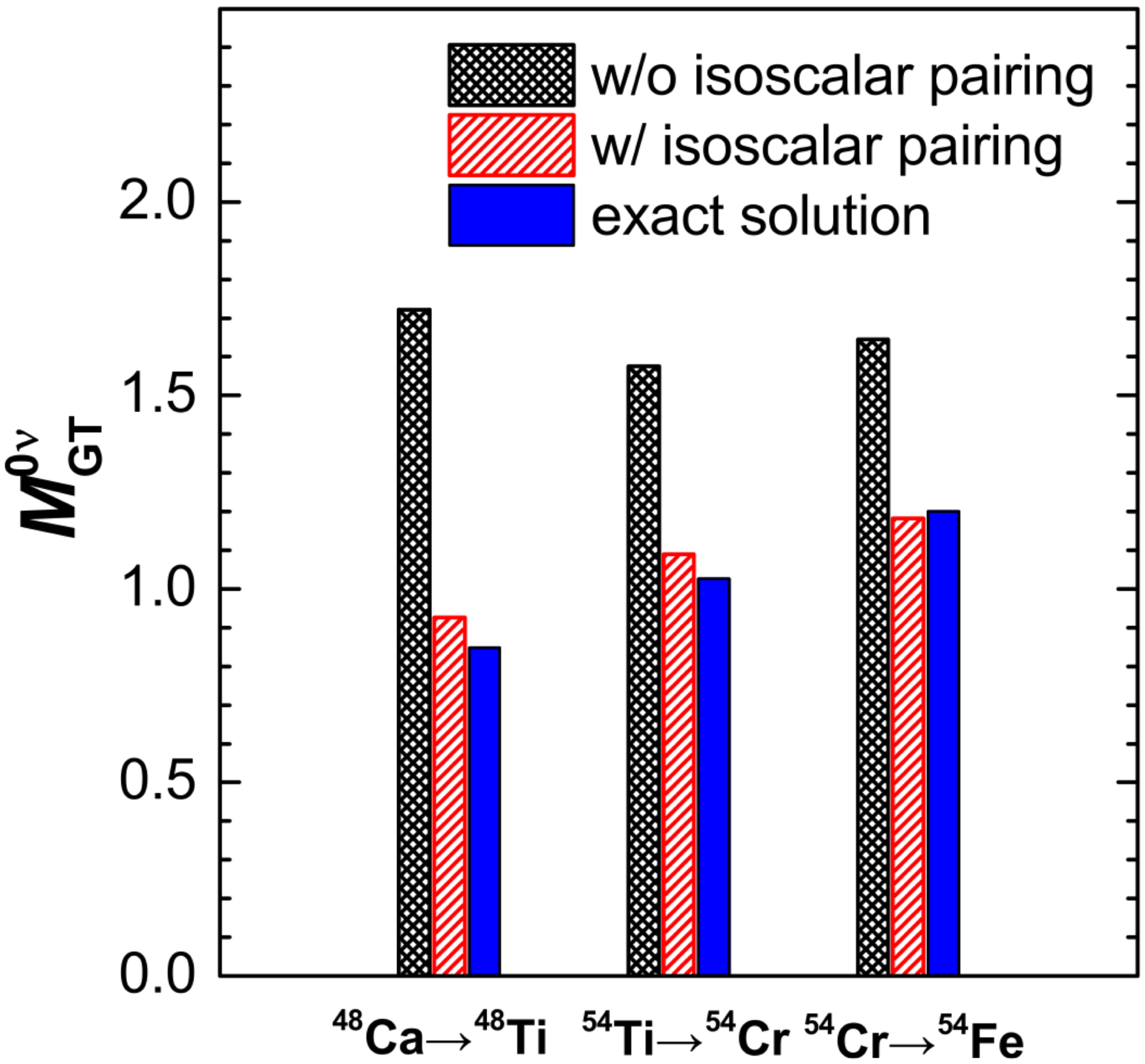
- Configuration mixing within GCM:

$$|\Psi^J_{NZ\sigma}\rangle = \sum_{K,q} f^{JK}_\sigma(q)|JMK;NZ;q\rangle$$

$$\sum_{K',q'}\{\mathcal{H}^J_{KK'}(q;q') - E^J_\sigma \mathcal{N}^J_{KK'}(q;q')\}f^{JK'}_\sigma(q') = 0$$

$$M^{0\nu\beta\beta}_\xi = \langle\Psi^{J=0}_{N_f Z_f}|\hat{O}^{0\nu\beta\beta}_\xi|\Psi^{J=0}_{N_i Z_i}\rangle$$

Level 1 GCM: Axial Shape and pn Pairing Fluctuation



We use the KB3G interaction for two GCM calculations:

- **Black column**: we set all the two-body matrix elements of the Hamiltonian with $J = 1$ and $T = 0$ to zero, because those are the ones which isoscalar pairing acts through.
  M_{GT} is overestimated.
- **Red column:** we use the full KB3G Hamiltonian:
  M_{GT} is suppressed, close to SM.

CFJ, J. Engel, and J.D. Holt, PRC 96, 054310 (2017)

Next Question:

Is shape + pn pairing correlations good enough?

So far so good, but ^{76}Ge/Se, ^{82}Se/Kr are well deformed. Quadrupole and pairing correlations may be predominant in this region.

What if we explore some heavier, near spherical or weakly deformed candidate nuclei?

Let's extend Hamiltonian-based GCM to ^{124}Sn/Te, ^{130}Te/Xe, and ^{136}Xe/Ba.

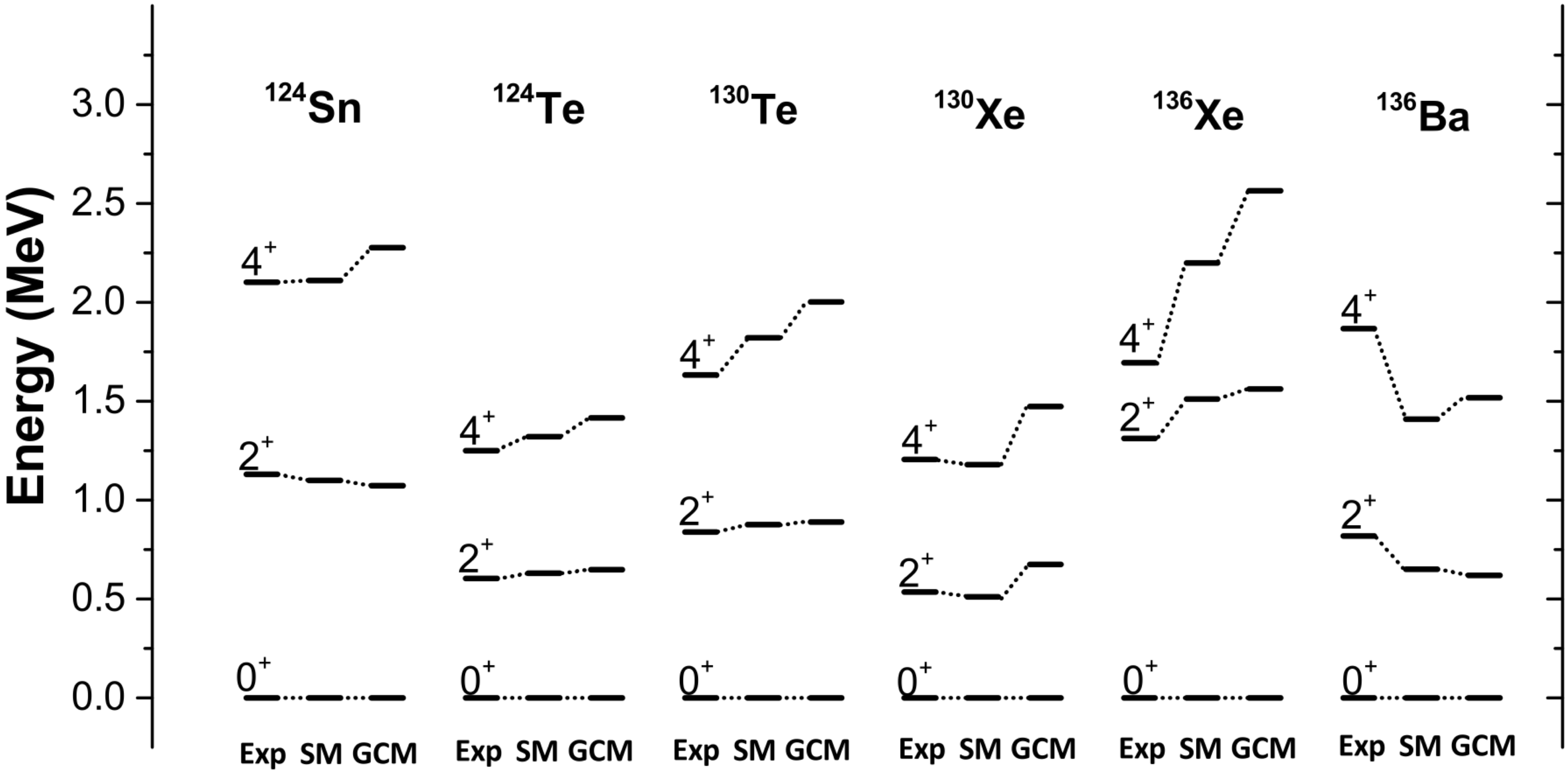
The SVD effective Hamiltonian within $0g_{7/2}$, $1d_{5/2}$, $1d_{3/2}$. $2s_{1/2}$, $0h_{11/2}$ orbits (*jj*55 model space) is employed

C. Qi and Z.X. Xu, PRC 86, 044323 (2012)

In addition, it's a stepping stone to even heavier $0\nu\beta\beta$ candidates (e.g., ^{150}Nd), for which no effective shell-model interaction exists.

Nuclear structure aspects

Low-lying level spectra



CFJ, M. Horoi, and A. Neacsu, PRC 98, 064324 (2018)

$0\nu\beta\beta$ Decay NME for Sn, Te, and Xe

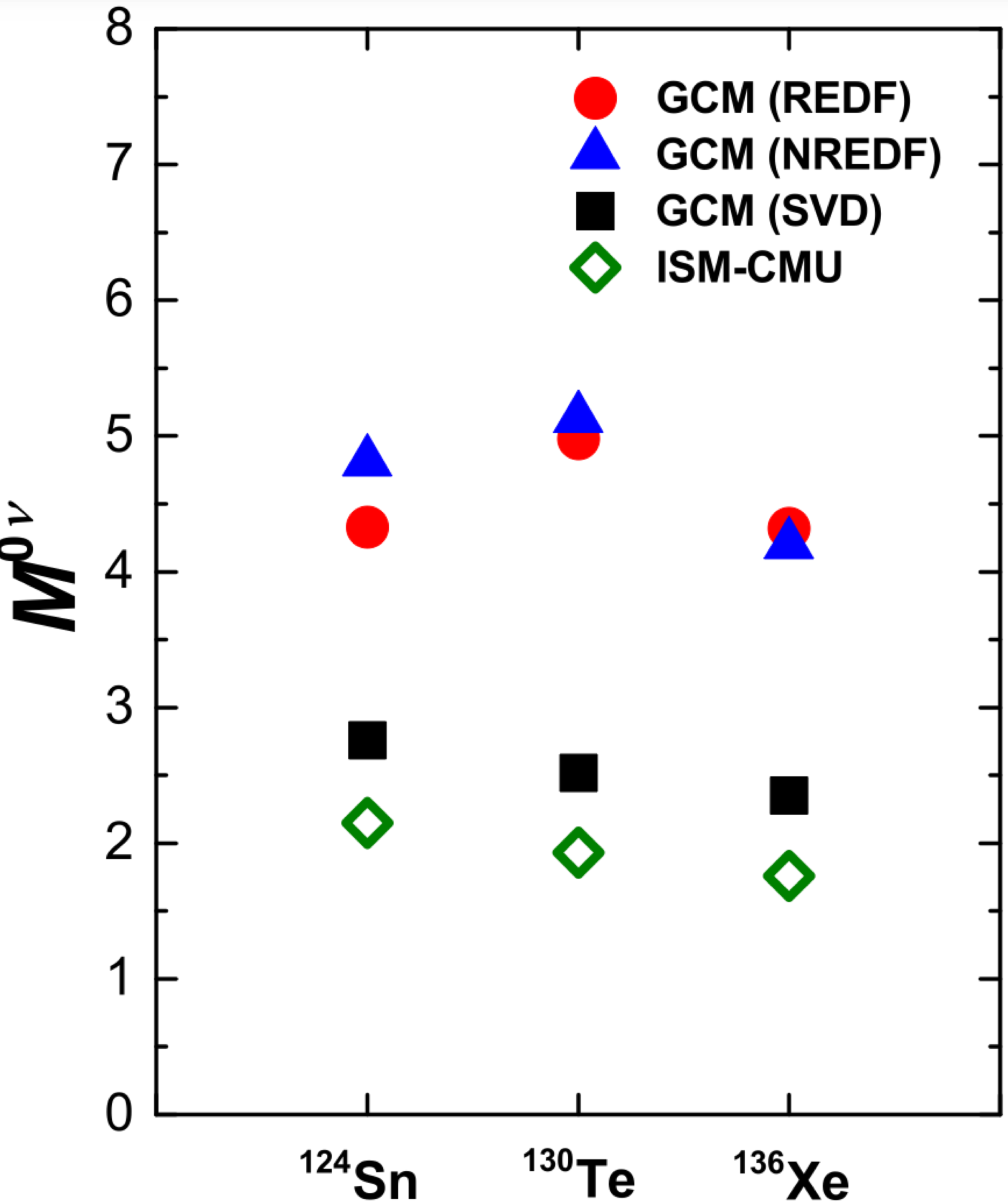


TABLE III. The NMEs obtained with SVD Hamiltonian by using GCM and SM for ^{124}Sn, ^{130}Te, and ^{136}Xe. The SM results are taken from Refs. [9,10]. CD-Bonn SRC parametrization was used.

		$M^{0\nu}_{\rm GT}$	$M^{0\nu}_{\rm F}$	$M^{0\nu}_{\rm T}$	$M^{0\nu}$
^{124}Sn	GCM	2.48	−0.51	−0.03	2.76
	SM	1.85	−0.47	−0.01	2.15
^{130}Te	GCM	2.25	−0.47	−0.02	2.52
	SM	1.66	−0.44	−0.01	1.94
^{136}Xe	GCM	2.17	−0.32	−0.02	2.35
	SM	1.50	−0.40	−0.01	1.76

Fermi part agrees well.
Gamow-Teller part is improved remarkably, but still ~30% overestimated.
WHY?

CFJ, M. Horoi, and A. Neacsu, PRC 98, 064324 (2018)

The Third question:

So shape + pn pairing correlations is not enough.
How to pin down all the correlations that are relevant?

Instead of guessing (albeit with good reasons) the important external fields for constrained HFB states, let's have the Hamiltonian itself tell us what to choose.

If we denote the GCM calculation above as "standard", here is where we branch from standard GCM…

The Third question:

Let's start from the Monte-Carlo shell model (MCSM).

- M. Honma, T. Mizusaki, and T. Otsuka, PRL 77, 3315 (1996)
- T. Otsuka, M. Honma, T. Mizusaki, *et al*. Prog. Part. Nucl. Phys. 47, 319 (2001)

The MCSM also uses non-orthogonal basis (HF) states. How does it choose states?

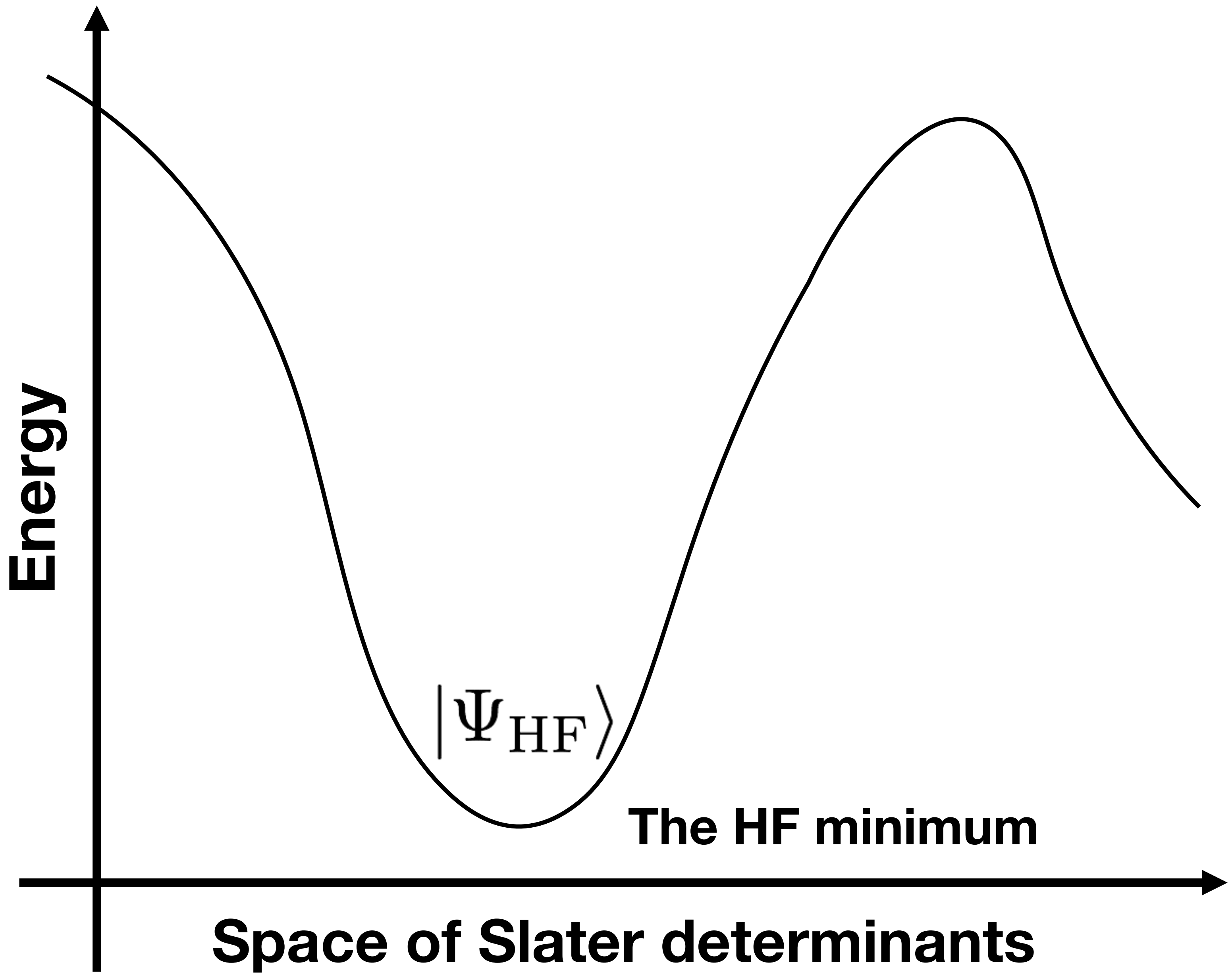
It exploits the Thouless theorem: the exponential of any one-body operator acting on a Slater determinant is another Slater determinant

$$\exp(\hat{Z})|\Psi\rangle = |\Psi'\rangle \equiv |\Psi(Z)\rangle$$

We can apply it to quasiparticle vacua, e.g., HFB state.

QTDA Equation

MCSM starts from the HF minimum

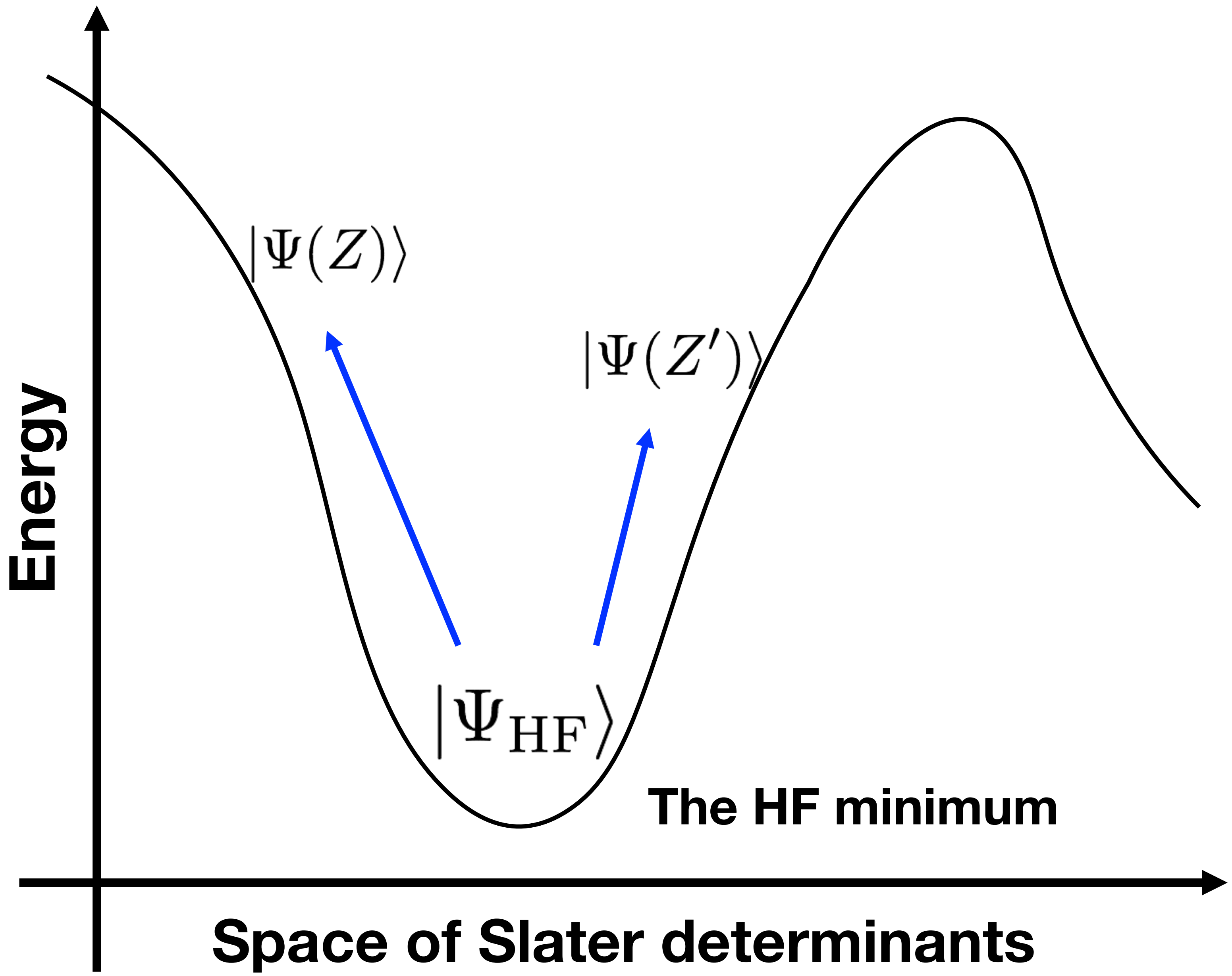


QTDA Equation

MCSM starts from the HF minimum

Apply Thouless evolution to explore the energy landscape

$$|\Psi(Z)\rangle = \exp(\hat{Z})|\Psi_{\mathrm{HF}}\rangle$$



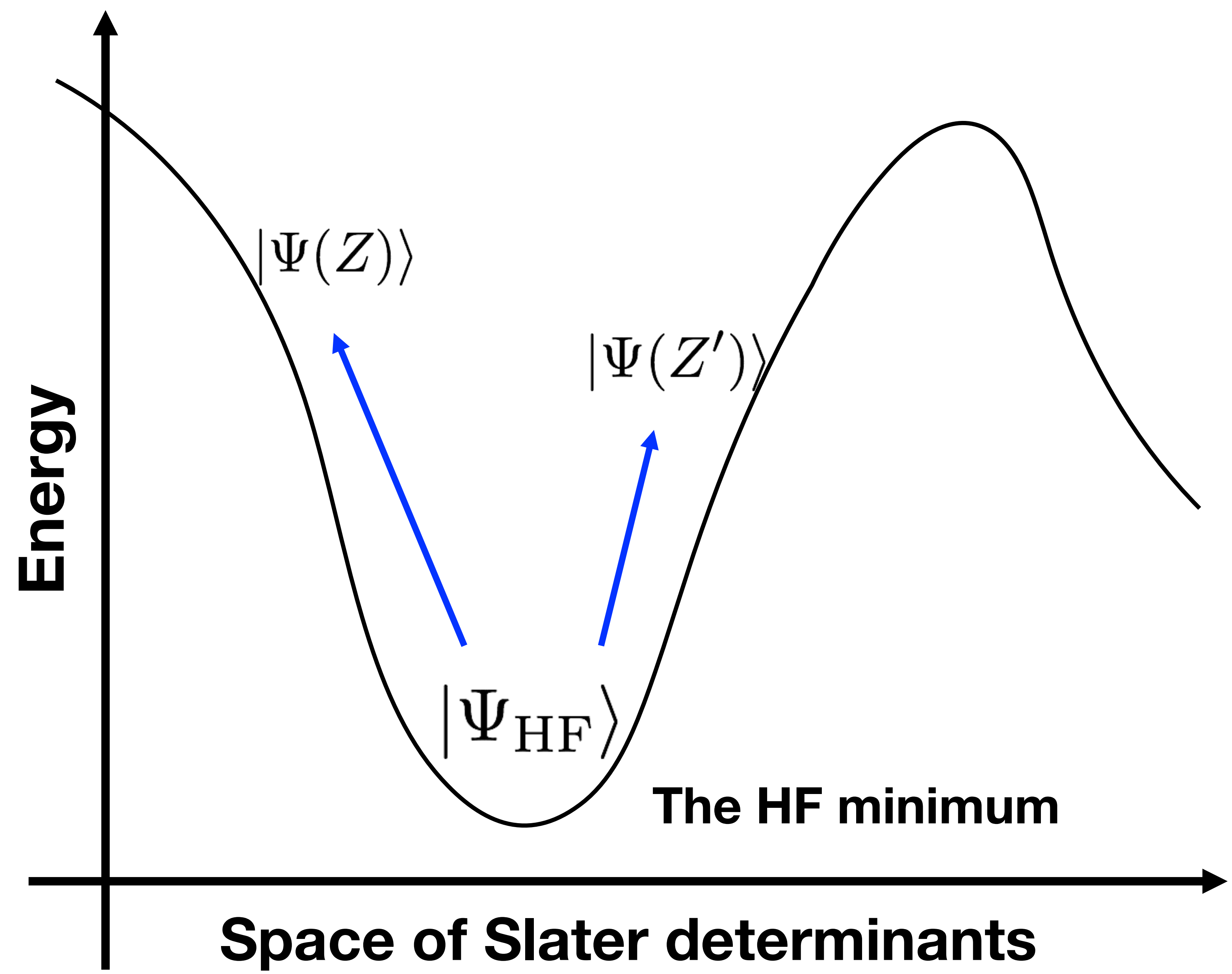
QTDA Equation

MCSM starts from the HF minimum

Apply Thouless evolution to explore the energy landscape

$$|\Psi(Z)\rangle = \exp(\hat{Z})|\Psi_{\mathrm{HF}}\rangle$$

$\hat{Z}$ Note that the curvature around HF minimum approximates the landscape as a quadratic in and thus a multi-dimensional harmonic oscillator, leading to TDA/RPA and their quasiparticle extension.



QTDA Equation and QTDA-evolved Basis

Here we don't adopt the full Monte Carlo machinery, just generate non-orthogonal states by applying Thouless evolution with QTDA operators.

Low-lying excited states are approximated as linear combinations

of two-quasiparticle excitations, represented by QTDA operator:

$$\hat{Z}_r = \frac{1}{2}\sum_{\alpha\alpha'} Z^r_{\alpha\alpha'}\hat{c}^\dagger_\alpha(0)\hat{c}^\dagger_{\alpha'}(0)$$

where $\hat{c}_\alpha(0) = \sum_\beta \hat{a}_\beta U^*_{\beta\alpha}(0) + \hat{a}^\dagger_\beta V^*_{\beta\alpha}(0)$

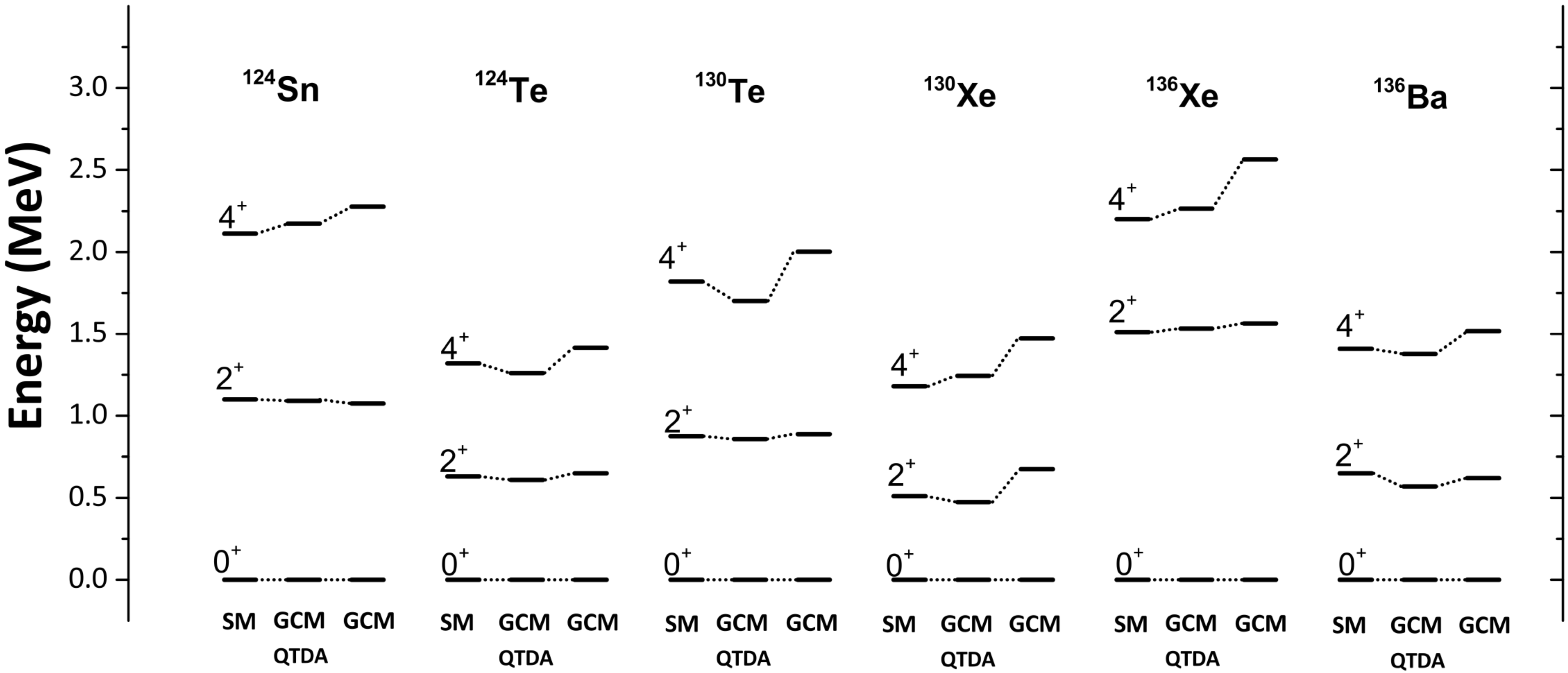
One computes the matrix elements of the Hamiltonian in a basis of two-quasiparticle excited states

$$A_{\alpha\alpha',\beta\beta'} = \langle\Phi_0|[\hat{c}_{\alpha'}(0)\hat{c}_\alpha(0), [\hat{H}, \hat{c}^\dagger_\beta(0)\hat{c}^\dagger_{\beta'}(0)]]|\Phi_0\rangle$$

We then solve $\sum_{\beta\beta'} A_{\alpha\alpha',\beta\beta'} Z^r_{\beta\beta'} = E^{\rm QTDA}_r Z^r_{\alpha\alpha'}$.

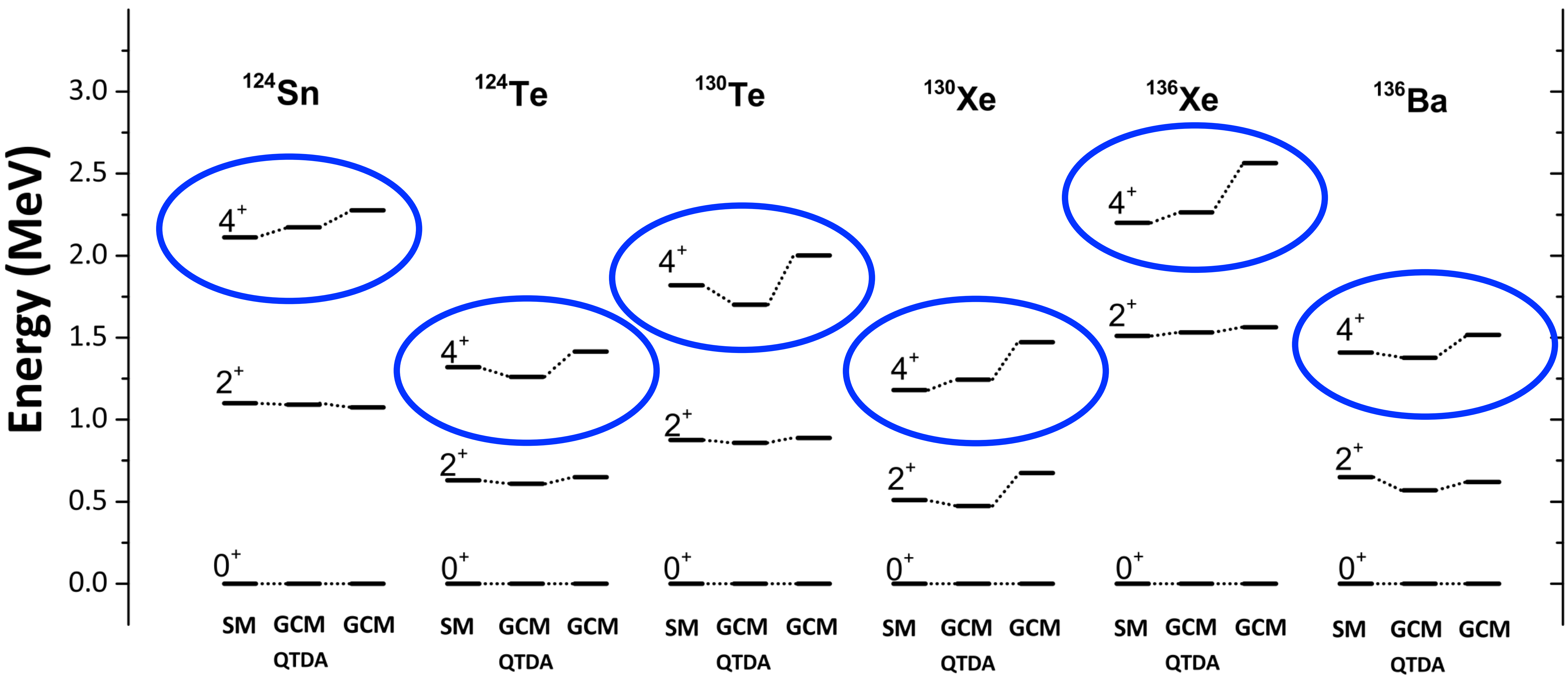
to find the coefficients of QTDA operator, and apply Thouless theorem to get a new state $|\Phi_r\rangle = \exp\left(\lambda\hat{Z}_r\right)|\Phi_0\rangle$

Comparison with standard GCM and SM



CFJ and Calvin W. Johnson, arXiv: 1908.01873 (2019)

Comparison with standard GCM and SM



Inclusion of the vibrational motion and two-quasiparticle configurations is important.

CFJ and Calvin W. Johnson, arXiv: 1908.01873 (2019)

Comparison with standard GCM and SM

TABLE I: The $B(E2 : 0_1^+ \to 2_1^+)$ (in e^2b^2) obtained with SVD Hamiltonian by using standard GCM [35], QTDA-driven GCM (this work), and SM [41, 42] for ^{124}Sn, ^{124}Te, ^{130}Te, ^{130}Xe, ^{136}Xe, and ^{136}Ba, compared to the adopted values [44].

	^{124}Sn	^{124}Te	^{130}Te	^{130}Xe	^{136}Xe	^{136}Ba
GCM (standard)	0.168	0.648	0.165	0.492	0.220	0.475
QTDA-GCM	0.137	0.547	0.145	0.415	0.180	0.418
SM	0.146	0.579	0.153	0.502	0.215	0.479
Adopted	0.162	0.560	0.297	0.634	0.217	0.413

CFJ and Calvin W. Johnson, arXiv: 1908.01873 (2019)

Comparison with standard GCM and SM

TABLE II: The nuclear matrix elements obtained with SVD Hamiltonian by using standard GCM[35], QTDA-driven GCM (this work), and SM [41, 42] for ^{124}Sn, ^{130}Te, and ^{136}Xe. CD-Bonn SRC parametrization was used.

		$M^{0\nu}_{\rm GT}$	$M^{0\nu}_{\rm F}$	$M^{0\nu}_{\rm T}$	$M^{0\nu}$
^{124}Sn	GCM (standard)	2.48	−0.51	−0.03	2.76
	QTDA-GCM	2.08	−0.73	−0.01	2.53
	SM	1.85	−0.47	−0.01	2.15
^{130}Te	GCM (standard)	2.25	−0.47	−0.02	2.52
	QTDA-GCM	1.97	−0.69	−0.01	2.39
	SM	1.66	−0.44	−0.01	1.94
^{136}Xe	GCM (standard)	2.17	−0.32	−0.02	2.35
	QTDA-GCM	1.65	−0.50	−0.01	1.96
	SM	1.50	−0.40	−0.01	1.76

CFJ and Calvin W. Johnson, arXiv: 1908.01873 (2019)

Next Steps from Here…

- Add many more reference states
  - We could add more QTDA phonons, or combine QTDA evolution with constrained HFB.
  - To reduce the computational burden, we should implement the efficient projection methods in the QTDA-driven GCM code.

- Calvin W. Johnson and Kevin D. O'Mara, PRC 96, 064304 (2017)
- Calvin W. Johnson and CFJ, JPG 46, 015101 (2019)

- One could try quasiparticle random phase approximation (QRPA) operators.
  - Incorporate two-particle two-hole components into the ground state, and hence improve the description of $0\nu\beta\beta$ decay NMEs.

Summary

- $0\nu\beta\beta$ decay is crucial probe for determining whether neutrinos are Majorana fermion.
- Developed a Hamiltonian-based GCM which treats triaxial shape and *pn* pairing correlations as coordinates. It enables treatment of systems presently unreachable by other methods.
- *Using vibration modes (e.g. QTDA) to build basis states around HFB shows improvement in nuclear structure aspects and $0\nu\beta\beta$ NMEs.*
- Both standard and QTDA-driven GCM can be further extended to other applications.