Hamiltonian-Based Generator Coordinate Method for Neutrinoless Double-β Decay







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standard model two-neutrino beta decay neutrinoless beta decay

Workshop on Neutrinoless double-beta decay, May 22nd @ Zhuhai, Guangdong

Baryogenesis through Leptogenesis

- Neutrino oscillation experiments ______ neutrinos have masses.
 Beyond the standard model.
- Neutrino masses are much less than charged leptons and quarks.
 Dirac masses from Higgs mechanism? Not likely.
- One solution: if neutrinos are Majorana fermions, i.e., their own antiparticles, the seesaw mechanism can introduce right-handed neutrinos with large Majorana masses.
- They decay into either leptons or anti-leptons via Yukawa couplings. The CP asymmetries of these decays result in lepton number asymmetry in the universe.



If this is true, neutrinos should be Majorana fermions. But how do we know that?

Probes: Neutrinoless Double-β Decay

ASTRONOMY SUPERIOR

In certain even-even nuclei, β decay is energetically forbidden, because m(Z, A) < m(Z+1, A), while double- β decay, from a nucleus of (Z, A) to (Z+2, A), is energetically allowed.

Isotope	$Q_{\beta\beta}$ (MeV)
⁷⁶ Ge	2.039
⁸² Se	2.992
¹⁰⁰ Mo	3.034
¹³⁰ Te	2.528
¹³⁶ Xe	2.468
¹⁵⁰ Nd	3.368









Allowed second-order weak process Maria Goeppert-Mayer (1935)

$2\nu\beta\beta$ observed for

⁴⁸Ca, ⁷⁶Ge, ⁸²Se, ⁹⁶Zr, ¹⁰⁰Mo, ¹¹⁶Cd, ¹²⁸Te, ¹³⁰Te, ¹³⁶Xe, ¹⁵⁰Nd



0v double- β decay ($0v\beta\beta$): $(Z, A) \rightarrow (Z+2, A) + 2e^{-1}$

- Tests lepton number conservation.
- The practical technique to determine if neutrinos might be Majorana particles.
- A method for determining the overall absolute neutrino mass scale



Ονββ Decay Experiments





CUORE





Collaboration	Isotope	Technique	mass (0νββ isotope)	Status	
CANDLES	Ca-48	305 kg CaF2 crystals - liq. scint	0.3 kg	Construction	
CARVEL	Ca-48	⁴⁸ CaWO ₄ crystal scint.	~ ton	R&D	
GERDA I	Ge-76	Ge diodes in LAr	15 kg	Complete	
GERDA II	Ge-76	Point contact Ge in LAr	31	Operating	
MAJORANA DEMONSTRATOR	Ge-76	Point contact Ge 25 kg		Operating	
LEGEND	Ge-76	Point contact	~ ton	R&D	
NEMO3	Mo-100 Se-82	Foils with tracking	king 6.9 kg 0.9 kg		
SuperNEMO Demonstrator	Se-82	Foils with tracking	7 kg	Construction	
SuperNEMO	Se-82	Foils with tracking	100 kg	R&D	
LUCIFER (CUPID)	Se-82	ZnSe scint. bolometer	18 kg	R&D	
AMoRE	Mo-100	CaMoO ₄ scint. bolometer	1.5 - 200 kg	R&D	
LUMINEU (CUPID)	Mo-100	ZnMoO ₄ / Li ₂ MoO ₄ scint. bolometer	1.5 - 5 kg	R&D	
COBRA	Cd-114,116	CdZnTe detectors	10 kg	R&D	
CUORICINO, CUORE-0	Te-130	TeO ₂ Bolometer	10 kg, 11 kg	Complete	
CUORE	Te-130	TeO ₂ Bolometer	206 kg	Operating	
CUPID	Te-130	TeO ₂ Bolometer & scint.	~ ton	R&D	
SNO+	Te-130	0.3% natTe suspended in Scint	160 kg	Construction	
EXO200	Xe-136	Xe liquid TPC	79 kg	Operating	
nEXO	Xe-136	Xe liquid TPC	~ ton	R&D	
KamLAND-Zen (I, II)	Xe-136	2.7% in liquid scint.	380 kg	Complete	
KamLAND2-Zen	Xe-136	2.7% in liquid scint.	750 kg	Upgrade	
NEXT-NEW	Xe-136	High pressure Xe TPC	5 kg	Operating	
NEXT	Xe-136	High pressure Xe TPC	100 kg - ton	R&D	
PandaX - 1k	Xe-136	High pressure Xe TPC	~ ton	R&D	
DCBA	Nd-150	Nd foils & tracking chambers	20 kg	R&D	

GERDA



MAJORANA



SNO+



Taken from J. F. Wilkerson's slides

Neutrino Mass Hierarchy

From neutrino oscillations we know $\Delta m_{sun}^2 \simeq 75 \text{ meV}^2 \qquad \Delta m_{atm}^2 \simeq 2400 \text{ meV}^2$ We also know the mixing angles that specify

the linear combinations of flavor eigenstates

$$m_{etaeta} \equiv \left|\sum_k m_k U_{ek}^2\right|$$

But we don't know the mass hierarchy.





A. Gando et al. PRL **117**, 082503 (2016)



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 $4.815(06) \times 10^{-15}$

 $1.469(05) \times 10^{-19}$

2017.85(64)^b

In case of process induced by light exchange, mass mechanism



J. Kotila and F. Iachello, PRC **85**, 034316 (2012)

In case of process induced by light exchange, mass mechanism





 $[T_{1/2}^{0\nu}]^{-1} = G_{0\nu}(Q,Z) |M_{0\nu}|^2 \langle m_{\beta\beta} \rangle^2$ Must be calculated by nuclear physics!

$$M^{0\nu} = M^{0\nu}_{\rm GT} - \frac{g_V^2}{g_A^2} M^{0\nu}_{\rm F} + M^{0\nu}_{\rm T}$$

with

$$\begin{split} M_{\rm GT}^{0\nu} &= \frac{2R}{\pi g_A^2} \int_0^\infty |q| d|q| \langle f| \sum_{a,b} \frac{j_0(|q|r_{ab})h_{\rm GT}(|q|)\vec{\sigma}_a \cdot \vec{\sigma}_b}{|q| + \bar{E} - (E_i + E_f)/2} \tau_a^+ \tau_b^+ |i\rangle \\ M_{\rm F}^{0\nu} &= \frac{2R}{\pi g_A^2} \int_0^\infty |q| d|q| \langle f| \sum_{a,b} \frac{j_0(|q|r_{ab})h_{\rm F}(|q|)}{|q| + \bar{E} - (E_i + E_f)/2} \tau_a^+ \tau_b^+ |i\rangle \\ M_{\rm T}^{0\nu} &= \frac{2R}{\pi g_A^2} \int_0^\infty |q| d|q| \langle f| \sum_{a,b} \frac{j_2(|q|r_{ab})h_{\rm T}(|q|)[3\vec{\sigma}_j \cdot \hat{r}_{ab}\vec{\sigma}_k \cdot \hat{r}_{ab} - \vec{\sigma}_a \cdot \vec{\sigma}_b}{|q| + \bar{E} - (E_i + E_f)/2} \tau_a^+ \tau_b^+ |i\rangle \end{split}$$

Lines of attack: * Construct effective operator.

* Find good initial and final ground-state wave functions: challenge for nuclear physics.



Nuclear Models: **QRPA, Shell model, GCM, etc.**



Current situation:

All the models miss important physics: omits correlations, omits single particle levels...

Some models are built on single independent-particle state.

Starting from one Slater determinant, e.g., the HF state $|\psi_0\rangle$, the ground state

$$|0\rangle = |\psi_0\rangle + \sum_{mi} C^0_{mi} a^{\dagger}_m a_i |\psi_0\rangle + \frac{1}{4} \sum_{mnij} C^0_{mn,ij} a^{\dagger}_m a^{\dagger}_n a_i a_j |\psi_0\rangle + \cdots$$

But exact diagonalization in complete Hilbert space is not solvable.

Protons









Some models are built on single independent-particle state.



Interacting shell model (ISM)

- Same starting point . $|0\rangle$
- Instead of solving Schrödinger equation in complete Hilbert space, one restricts the dynamics in a configuration space.

$$H|\Phi_i\rangle = E_i|\Phi_i\rangle \to H_{\text{eff}}|\bar{\Phi}_i\rangle = E_i|\bar{\Phi}_i\rangle$$

Configuration interaction of orthonormal Slater determinants:

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

Diagonalizing the H_{eff} in the
orthonormal basis.





Review of Different Nuclear Models

Some models are built on single independent-particle state.

Interacting shell model (ISM)

Pros:

 Arbitrarily complex correlations within the model space.

Cons:

- Relatively small configuration spaces.
 - At present most of the 0vββ decay NME calculations carried out by SM are limited in one single 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.



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

Generator-Coordinate Method (GCM)



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

However, the results of GCM based on energy density functional look different from the ones given by the SM calculations.



Both the shell model and the EDF-based GCM could be missing important physics.

- The EDF-GCM omits correlations.
- The shell model omits many singleparticle levels.

Does the discrepancy come from methods themselves, or the interactions they use?



Let's combine the virtues of both frameworks through an idealistic GCM that includes all the important correlations in a large single-particle space!

Sure. My current achievement is the first step in this direction: Developed a Hamiltonian-based GCM in one and two (and possibly more) shells.

More correlations, larger space.

Another way is IM-SRG + GCM (IM-GCM), c.f. Jiangming Yao's talk...

Generator Coordinate Method

- Using a realistic effective Hamiltonian.
- * We are trying to include all possible collective correlations.

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

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

- HFB states $|\Phi(q)\rangle$ with multipole constraints $\langle H' \rangle = \langle H_{\text{eff}} \rangle - \lambda_Z(\langle N_Z \rangle - Z) - \lambda_N(\langle N_N \rangle - N) - \sum \lambda_i(\langle \mathcal{O}_i \rangle - q_i),$
- * 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:

Ονββ ΝΛ

$$\begin{aligned} & \mathsf{GCM wavefunction:} \quad |\Psi_{NZ\sigma}^{J}\rangle = \sum_{K,q} f_{\sigma}^{JK}(q) | JMK; NZ; q \rangle \\ & \mathsf{Hill-Wheeler equation:} \ \sum_{K',q'} \{\mathcal{H}_{KK'}^{J}(q;q') - E_{\sigma}^{J}\mathcal{N}_{KK'}^{J}(q;q')\} f_{\sigma}^{JK'}(q') = 0 \end{aligned}$$

AE:
$$M_{\xi}^{0\nu\beta\beta} = \langle \Psi_{N_{f}Z_{f}}^{J=0} | \hat{O}_{\xi}^{0\nu\beta\beta} | \Psi_{N_{i}Z_{i}}^{J=0} \rangle$$

Generator Coordinate Method





The first 2⁺-state energies and B(E2) given by Hamiltonian-based GCM are in great agreement with SM results.



Q1: Which correlations are the most relevant to $0v\beta\beta$ NMEs?



T. Rodriguez and G. Martinez-Pinedo PRL **105**, 252503 (2010)

N. Hinohara and J. Engel PRC **90**, 031301(R) (2014)

Generator Coordinate Method



Proton-neutron pairing





Triaxial deformation



~10% reduced if triaxial-shape fluctuation is included.

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



Q2: What is the effect from enhancement of model space?

For the first time, we work in the full fp-sdg two-shell space, which is **unreachable** by shell model.

- The effective fp-sdg-shell interaction calculated by EKK perturbative method.
- The three-body part is reduced to an effective two-body force by summing the third particle over a set of occupied states (⁵⁶Ni here).

TABLE II. GCM results for the Gamow-Teller $(M_{GT}^{0\nu})$, Fermi $(M_F^{0\nu})$, and tensor $(M_T^{0\nu}) 0\nu\beta\beta$ matrix elements for the decay of ⁷⁶Ge in two shells, without and with triaxial deformation.

	Axial	Triaxial
$M_{ m GT}^{0 u}$	3.18	1.99
$-rac{g_V^2}{g_A^2}M_{ m F}^{0 u}$	0.55	0.38
$M_{\mathrm{T}}^{0 u}$	-0.01	-0.02
Total $M^{0\nu}$	3.72	2.35

Enhanced axially-deformed result: Larger space captures more like-particle pairing.

Reduced triaxially-deformed result: Larger space captures more effect from triaxial deformation.







Q3: Is shape + pn pairing correlations good enough?



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

		$M_{ m GT}^{0 u}$	$M_{ m F}^{0 u}$	$M_{ m T}^{0 u}$	$M^{0 u}$
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?





I-pair decomposition:

Decomposition of the NMEs over the angular momentum / of the proton (or neutron) pairs, that is

$$M^{0\nu}_{\alpha} = \sum_{I} M^{0\nu}_{\alpha}(I)$$

where $M^{0\nu}_{\alpha}(I)$ represent the contribution from each pair-spin / to the part of the NME.

- GCM reproduces well the cancellation between the /= 0 and /= 2 contributions.
- * GCM barely produce any contributions with $l \ge 4$.





Ονββ Decay NME for Sn, Te, and Xe







Q4: So shape + pn pairing correlations is not enough. How to pin down all the correlations that are relevant?

I proposed a novel idea to incorporate important correlations in GCM.

Starts from the HF minimum.

Apply Thouless evolution to explore the energy landscape

Thouless theorem:

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



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Space of Slater determinants



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Difine an energy landscape $E(Z) = \langle \Psi(Z) | \hat{H} | \Psi(Z) \rangle$ which can be expanded in Z. Note that the curvature around HF minimum approximates the landscape as a quadratic in Z and thus a multi-dimensional harmonic oscillator, leading to TDA/RPA and their quasiparticle extension.



Here we generate non-orthogonal states by applying Thouless evolution with QTDA operators.

Low-lying excited states are approximated as linear combinations of twoquasiparticle excitations, represented by QTDA operator:

$$\hat{Z}_r = \frac{1}{2} \sum_{\alpha \alpha'} Z^r_{\alpha \alpha'} \hat{c}^{\dagger}_{\alpha}(0) \hat{c}^{\dagger}_{\alpha'}(0) \qquad \text{where} \quad \hat{c}_{\alpha}(0) = \sum_{\beta} \hat{a}_{\beta} U^*_{\beta \alpha}(0) + \hat{a}^{\dagger}_{\beta} V^*_{\beta \alpha}(0)$$

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

quasiparticle excited states

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

We then solve $\sum_{\beta\beta'} A_{\alpha\alpha',\beta\beta'} Z_{\beta\beta'}^r = E_r^{\text{QTDA}} Z_{\alpha\alpha'}^r$. to find the coefficients $Z_{\alpha\alpha'}^r$ of QTDA operator, and apply Thouless theorem to get a new state

 $|\Phi_r
angle = \exp\left(\lambda \hat{Z}_r
ight)|\Phi_0
angle$





		$M_{ m GT}^{0 u}$	$M_{ m F}^{0 u}$	$M_{ m T}^{0 u}$	$M^{0 u}$
¹²⁴ Sn	CHFB-GCM	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	CHFB-GCM	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	CHFB-GCM	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

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

CFJ and C.W. Johnson, PRC 100, 031303(R) (2019)



Q5: How about the effect from the tensor force? Considering that it has a robust effect on the single-particle energies of nuclei





CFJ and C. X. Yuan, in preparation.



NMEs are suppressed, why?





Enhanced quadrupole deformation.

Enhanced isoscalar pairing.

CFJ and C. X. Yuan, in preparation.





Neutron and proton effective single-particle energies at spherical shape relative to $2s_{1/2}$ orbit.



Change in proton occupancies and neutron vacancies

CFJ and C. X. Yuan, in preparation.



- Summary
 - 0νββ decay is crucial probe for determining whether neutrinos are Majorana fermion.
 - Hamiltonian-based GCM 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.

Next Steps from Here...

- More reference states
 - More QTDA phonons, or combine QTDA evolution with constrained HFB.
- ✤ Quasiparticle random phase approximation (QRPA) operators.
- Effective Hamiltonian in larger space, or from *ab initio* non-perturbative method.
 - ♦ Target nuclei: ⁹⁶Zr, ¹⁰⁰Mo, ¹¹⁶Cd, ¹⁵⁰Nd...

In Collaboration with...

ASTRONOUT SHALL BE

- Jiangming Yao, SYSU
- Ning Li, SYSU
- Cenxi Yuan, SYSU
- Jonathan Engel, UNC
- Calvin W. Johnson, SDSU
- Jason D. Holt, TRIUMF
- Mihai Horoi, CMU
- Nobuo Hinohara, U of Tsukuba
- Javier Menendez, U of Barcelona



Thanks for your attention!

HAPEL Y