Multi-particle-hole configurations in description of double beta decay

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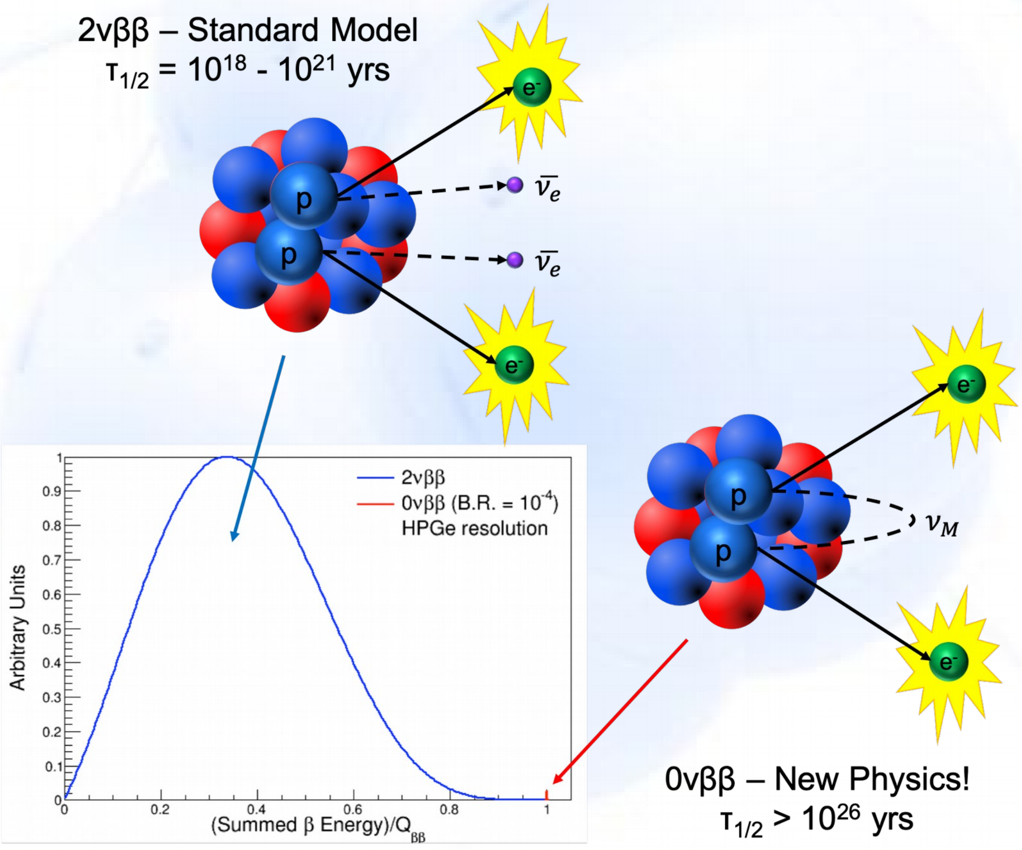
Motivation

Double Beta Decay is so interesting physical phenomenon because: **Particle** & **Nuclear** & **Atomic** physics meet here. It is perfect laboratory to test validity of **SM** (2νββ) and search for effects **beyond SM** physics (0νββ). It can provide us more information about least understood elementary particle (**neutrino**). It is **challenge** for **experimental physics** – the **slowest decay** process in the universe.

How **theoretical nuclear physics** can contribute to the effort of understanding the Double Beta Decay?

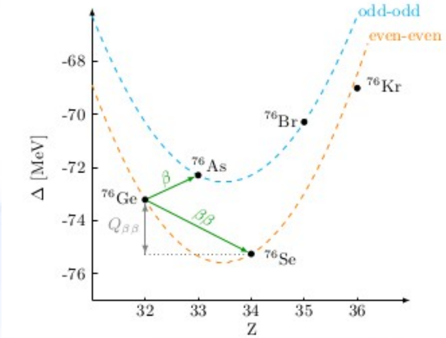
Outline of the Seminar:

- **Double β decay & neutrino physics.**
- **Double β decay & nuclear physics.**
- **Beyond 1p – 1h nuclear methods.**
- **Preliminary results.**
- **Summary & Outlook.**



Double β decay & neutrino physics

Existence of double β decay proposed by **Maria Goeppert Mayer** in 1935. In its standard variant, **2 electrons + 2 (anti)neutrinos** are emmitted (**2νββ**).
Decay occurs in nuclei where single β decay is not energetically allowed.



There are 35 naturally occuring isotopes capable of **2νββ**.
2νββ or double electron capture confirmed experimentaly in 14 isotopes.

Isotope	$T_{1/2}(2\nu)$, yr	$\mid M^{eff}_{2\nu}\mid$ ($G_{2\nu}$ from [24])	$\mid M^{eff}_{2\nu}\mid$ ($G_{2\nu}$ from [25])	Recommended Value
$2\nu\beta\beta$:				
^{48}Ca	$5.3^{+1.2}_{-0.8}\cdot 10^{19}$	$0.0348^{+0.0030}_{-0.0034}$	$0.0348^{+0.0030}_{-0.0034}$	0.035 ± 0.003
^{76}Ge	$(1.88\pm 0.08)\cdot 10^{21}$	$0.1051^{+0.0023}_{-0.0024}$	$0.1074^{+0.0024}_{-0.0022}$	0.106 ± 0.004
^{82}Se	$0.87^{+0.02}_{-0.01}\cdot 10^{20}$	$0.0849^{+0.0005}_{-0.0010}$	$0.0855^{+0.0005}_{-0.0010}$	0.085 ± 0.001
^{96}Zr	$(2.3\pm 0.2)\cdot 10^{19}$	$0.0798^{+0.0037}_{-0.0032}$	$0.0804^{+0.0038}_{-0.0033}$	0.080 ± 0.004
^{100}Mo	$7.06^{+0.15}_{-0.13}\cdot 10^{18}$	$0.2071^{+0.0019}_{-0.0022}$	$0.2096^{+0.0020}_{-0.0022}$	
		$0.1852^{+0.0017}_{-0.0019}$ (a)		0.185 ± 0.002
^{100}Mo-^{100}Ru(0^+_1)	$6.7^{+0.5}_{-0.4}\cdot 10^{20}$	$0.1571^{+0.0048}_{-0.0056}$	$0.1619^{+0.0050}_{-0.0058}$	
		$0.1513^{+0.0047}_{-0.0053}$ (a)		0.151 ± 0.005
^{116}Cd	$(2.69\pm 0.09)\cdot 10^{19}$	$0.1160^{+0.0020}_{-0.0019}$	$0.1176^{+0.0020}_{-0.0019}$	
		$0.1084^{+0.0024}_{-0.0019}$ (a)		0.108 ± 0.003
^{128}Te	$(2.25\pm 0.09)\cdot 10^{24}$	$0.0406^{+0.0008}_{-0.0008}$	$0.0454^{+0.0009}_{-0.0009}$	0.043 ± 0.003
^{130}Te	$(7.91\pm 0.21)\cdot 10^{20}$	$0.0288^{+0.0004}_{-0.0004}$	$0.0297^{+0.0004}_{-0.0004}$	0.0293 ± 0.0009
^{136}Xe	$(2.18\pm 0.05)\cdot 10^{21}$	$0.0177^{+0.0002}_{-0.0002}$	$0.0184^{+0.0002}_{-0.0002}$	0.0181 ± 0.0006
^{150}Nd	$(9.34\pm 0.65)\cdot 10^{18}$	$0.0543^{+0.0020}_{-0.0018}$	$0.0550^{+0.0020}_{-0.0018}$	0.055 ± 0.003
^{150}Nd-^{150}Sm(0^+_1)	$1.2^{+0.3}_{-0.2}\cdot 10^{20}$	$0.0438^{+0.0042}_{-0.0046}$	$0.0450^{+0.0043}_{-0.0048}$	0.044 ± 0.005
^{238}U	$(2.0\pm 0.6)\cdot 10^{21}$	$0.1853^{+0.0361}_{-0.0227}$	$0.0713^{+0.0139}_{-0.0088}$	$0.13^{+0.09}_{-0.07}$
ECEC(2ν):				
^{78}Kr (b)	$1.9^{+1.3}_{-0.8}\cdot 10^{22}$	$0.2882^{+0.0829}_{-0.0706}$ [105]	$0.3583^{+0.1126}_{-0.0822}$	$0.32^{+0.15}_{-0.11}$
^{124}Xe (b)	$(1.8\pm 0.5)\cdot 10^{22}$	$0.0568^{+0.0101}_{-0.0650}$ [105]	$0.0607^{+0.0107}_{-0.0070}$	$0.059^{+0.013}_{-0.009}$
^{130}Ba	$(2.2\pm 0.5)\cdot 10^{21}$	$0.1741^{+0.0239}_{-0.0170}$ [105]	$0.1754^{+0.0241}_{-0.0171}$	$0.175^{+0.024}_{-0.017}$

2νββ half-lifes

Table from **A. Barabash**, *Universe 6*, 159, (2020).

$$T^{-1}_{1/2} = G_{2\nu}\cdot g_A^4\cdot \underbrace{(m_e c^2\cdot M_{2\nu})^2}_{\text{effective nuclear transition amplitude}},$$

phase space integration

effective nuclear transition amplitude

Double β decay & neutrino physics

Double β decay can open a window for better understanding of **particle (neutrino)** physics, mechanisms of **mass generation** and physics **beyond Standard Model**.

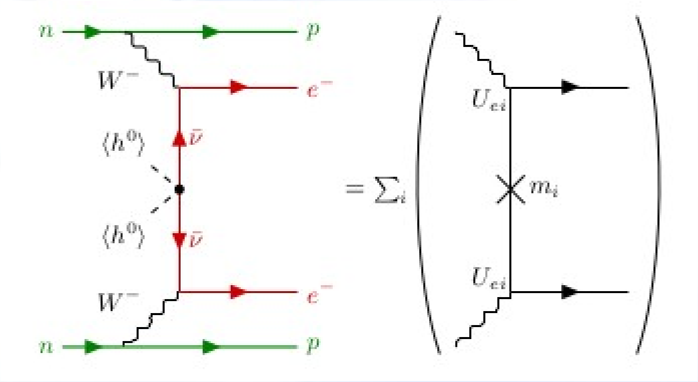
$$\frac{1}{T^{0\nu}_{1/2}} = \left|\frac{m_{\beta\beta}}{m_e}\right|^2 g_A^4 \left|M^{0\nu}(g_A)\right|^2 G^{0\nu}$$

neutrino mass

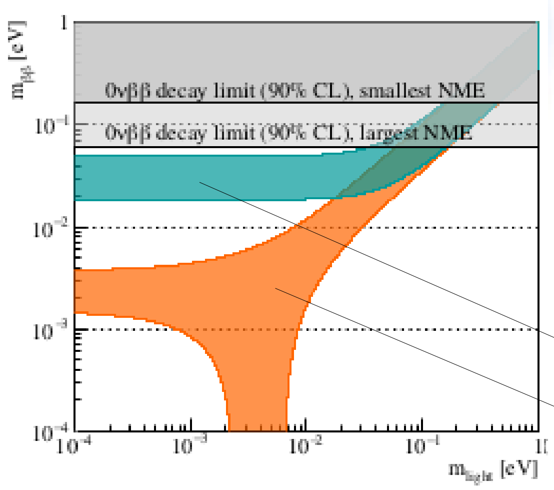
effective nuclear transition amplitudes

phase space integration

0νββ half-life depends on neutrino masses



Figs. from *M. Agostini et al.*, **ArXiv:2202.01787v2**



Normal versus **inverted hierarchy** of neutrino mass ordering. Experiments could distinguish these variants.

inverted mass hierarchy

normal mass hierarchy

If **0νββ** exists → neutrinos **Majorana** instead of **Dirac** fermions.

violation of lepton number. Connected with some processes of **leptogenesis**?

Double β decay & nuclear physics

Nuclear transition amplitudes (**NME**):

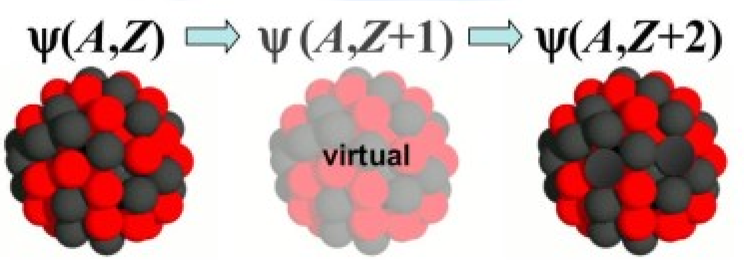
2νββ

daughter **intermediate** **mother** nucleus

$$M^{2\nu}_{F,GT} = \sum_n \frac{\langle f \parallel \mathcal{O}_{F,GT} \parallel J_n^+\rangle\langle J_n^+ \parallel \mathcal{O}_{F,GT} \parallel i\rangle}{E_n - (E_i + E_f)/2}$$

Fermi op. **Gamow-Teller** op.

$$\mathcal{O}_F = \sum_{k=1}^{A} \tau_k^+, \qquad \mathcal{O}_{GT} = \sum_{k=1}^{A} \tau_k^+ \sigma_{\mathbf{k}}.$$



NME's calculated within various* nuclear structure methods vary a lot among each other. It is not very satisfactory for predictions of half-lifes.

* **EDF, IBM, QRPA, Shell Model, In-Medium SRG, Coupled Cluster**

0νββ

$$M^{0\nu} = M^{0\nu}_{GT} - M^{0\nu}_F / g_A^2 + M^{0\nu}_T$$

closure approximation is assumed here

$$M^{0\nu}_F = \sum_{r,s} \langle f | h_F(r_-, \bar{E}_n) \tau_r^+ \tau_s^+ | i \rangle ,$$
$$M^{0\nu}_{GT} = \sum_{r,s} \langle f | h_{GT}(r_-, \bar{E}_n) \tau_r^+ \tau_s^+ \vec{\sigma}_r \cdot \vec{\sigma}_s | i \rangle ,$$
$$M^{0\nu}_T = \sum_{r,s} \langle f | h_T(r_-, \bar{E}_n) \tau_r^+ \tau_s^+ \left(3(\vec{\sigma}_r \cdot \hat{\mathbf{r}}_-)(\vec{\sigma}_s \cdot \hat{\mathbf{r}}_-) - \vec{\sigma}_r \cdot \vec{\sigma}_s\right) | i \rangle$$

In **0νββ** we work with **2-body NME**.

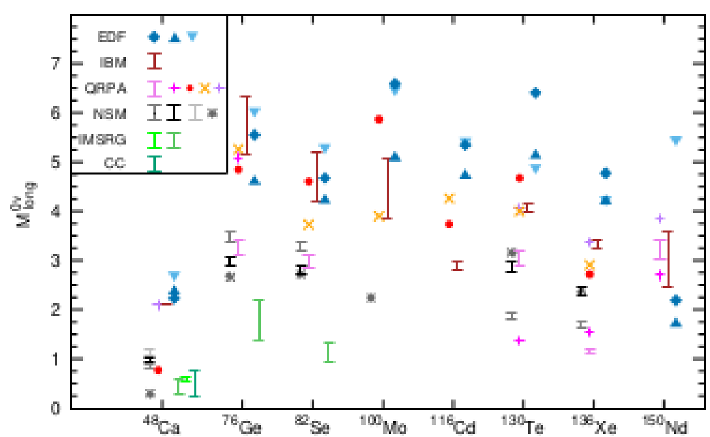
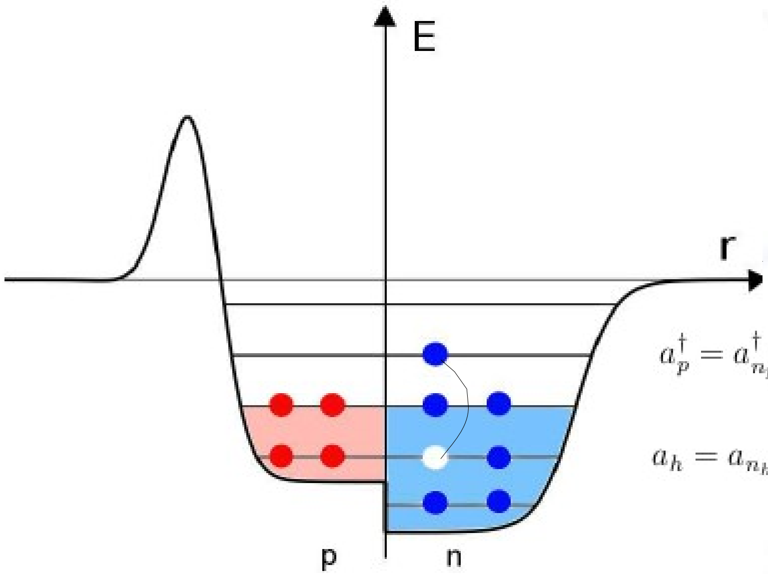


Fig. from *M. Agostini et al.*, **ArXiv:2202.01787v2**

Mean Field & 1particle-1hole exc.

Mean Field: Obtaining mean field by solving **Hartree-Fock (HF) method**.
The **residual interaction** must be taken back into accout.



$a_p^\dagger = a^\dagger_{n_p l_p m_p s_p}$

$a_h = a_{n_h l_h m_h s_h}$

How to represent **excitations**?

particle-hole configurations.

$$a_p^\dagger a_h |HF\rangle = a_p^\dagger a_h |\Psi\rangle$$

… creation in “particle“ level

… annihilation in “hole“ level

Methods to describe **nuclear excitation spectra** which are based on **1particle-1hole** configurations:

Tamm Dancoff Approximation (**TDA**) & Random Phase Approximation (**RPA**)

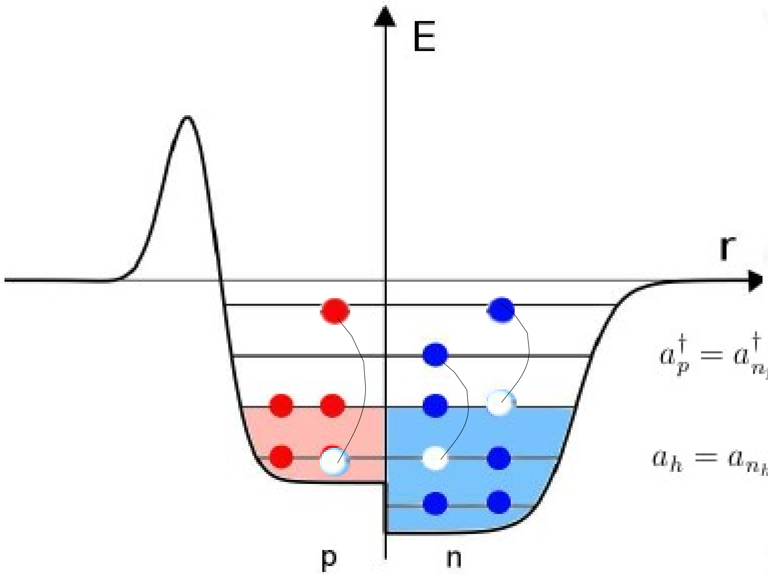
from **HF** state

from (implicitly) **correlated** state

Mean Field & *n* particle- *n* hole exc.

Beyond Mean Field: We can introduce 1p-1h, 2p-2h, 3p-3h … excitations.

Can we proceed in some general way?
1**p**-1**h,** 2**p**-2**h**, 3**p**-3**h**, … , n**p**-n**h** excitations.



$a_p^\dagger = a^\dagger_{n_p l_p m_p s_p}$

$a_h = a_{n_h l_h m_h s_h}$

Hilbert space – divided into subspaces

$$\mathcal{H} = \mathcal{H}_0 \oplus \mathcal{H}_1 \oplus \mathcal{H}_2 \oplus \ldots \oplus \mathcal{H}_n$$

HF – Hartree-Fock state (nucleons occupy lowest single-particle levels)
1p-1h = 1**particle** – 1**hole** excitation of HF
2p-2h = 2**particle** – 2**hole** excitation of HF
.
.
np-nh = n**particle** – n**hole** excitation of HF

Methods for (1**p**-1**h,** 2**p**-2**h**):
Second TDA, **Second RPA**

Methods for general n**p**-n**h** :
Equation of Motion Phonon Method (EMPM)

Second TDA & RPA

In **Hartree-Fock** (HF) we obtain optimized **single-particle basis** & reference state **HF vacuum** |HF>

Excited states – generally superpositions of **1particle-1hole** configurations in **TDA, RPA**
(1particle-1hole + 2particle-2hole) configurations in **second TDA**, **second RPA**

formalism of **phonons** (collective excitations):

$$[\boldsymbol{H}_{intr}, \boldsymbol{Q}_\nu^\dagger]|0\rangle \equiv \hbar\omega_\nu \boldsymbol{Q}_\nu^\dagger|0\rangle$$

$$|\nu\rangle = \boldsymbol{Q}_\nu^\dagger|0\rangle, \quad \boldsymbol{Q}_\nu|0\rangle = 0$$

random phase approximation (**RPA**): 1p-1h excitations from implicitly **correlated ground state** |0> $\neq$ |HF>

$$Q_\nu^{\dagger(\mathrm{RPA})} = \sum_{ph}(X_{ph}^\nu a_p^\dagger a_h - Y_{ph}^\nu a_h^\dagger a_p)$$

Tamm-Dancoff approximation (**TDA**): 1p-1h excitations from HF (|0> = |HF>) **no correlation** in ground state (**Y^ν_{ph} = 0**).

$$Q_\nu^{\dagger(\mathrm{TDA})} = \sum_{ph} X_{ph}^\nu a_p^\dagger a_h$$

second RPA (**SRPA**): extension of RPA accounting for **2p-2h excitations**

$$Q_\nu^{\dagger(\mathrm{SRPA})} = \sum_{ph}(X_{ph}^{\nu(1)} a_p^\dagger a_h - Y_{ph}^{\nu(1)} a_h^\dagger a_p) + \sum_{p_1p_2h_1h_2}(X_{p_1p_2h_1h_2}^{\nu(2)} a_{p_1}^\dagger a_{p_2}^\dagger a_{h_1} a_{h_2} - Y_{p_1p_2h_1h_2}^{\nu(2)} a_{h_1}^\dagger a_{h_2}^\dagger a_{p_1} a_{p_2})$$

Second TDA (**STDA**): $$Q_\nu^{\dagger(\mathrm{STDA})} = \sum_{ph} X_{ph}^{\nu(1)} a_p^\dagger a_h + \sum_{p_1p_2h_1h_2} X_{p_1p_2h_1h_2}^{\nu(2)} a_{p_1}^\dagger a_{p_2}^\dagger a_{h_1} a_{h_2}$$

Second TDA & RPA

Matrix form of SRPA:

$$\left(\begin{array}{cc|cc} A & A_{12} & B & B_{12} \\ A_{21} & A_{22} & B_{21} & B_{22} \\ \hline -B^* & -B^*_{12} & -A^* & -A^*_{12} \\ -B^*_{21} & -B^*_{22} & -A^*_{21} & -A^*_{22} \end{array}\right)\left(\begin{array}{c} X^{\nu\,(1)} \\ X^{\nu\,(2)} \\ \hline Y^{\nu\,(1)} \\ Y^{\nu\,(2)} \end{array}\right) = \hbar\omega_{\nu}^{SRPA}\left(\begin{array}{c} X^{\nu\,(1)} \\ X^{\nu\,(2)} \\ \hline Y^{\nu\,(1)} \\ Y^{\nu\,(2)} \end{array}\right)$$

Quasiboson approximation

C. Yannouleas, Phys. Rev. C ***35****, 1159 (1987)*

$$(A)_{ph,p'h'} \approx \langle HF|\left[a_h^\dagger a_p,\left[H_{intr}, a_{p'}^\dagger a_{h'}\right]\right]|HF\rangle$$

$$(B)_{ph,p'h'} \approx -\langle HF|\left[a_h^\dagger a_p,\left[H_{intr}, a_{h'}^\dagger a_{p'}\right]\right]|HF\rangle$$

$$(A_{12})_{ph,\,p_1p_2h_1h_2} \approx \langle HF|\left[a_h^\dagger a_p,\left[H_{intr}, a_{p_1}^\dagger a_{p_2}^\dagger a_{h_2} a_{h_1}\right]\right]|HF\rangle$$

$$(A_{22})_{p_1h_1p_2h_2,\,p_1'h_1'p_2'h_2'} \approx \langle HF|\left[a_{h_1}^\dagger a_{h_2}^\dagger a_{p_1} a_{p_2},\left[H_{intr}, a_{p_2'}^\dagger a_{p_1'}^\dagger a_{h_2'} a_{h_1'}\right]\right]|HF\rangle$$

For 2-body Hamiltonian and HF reference state → QBA → B_{12}, B_{21}, B_{22} =0
No explicit mixing between $|HF\rangle$ and $|2p2h\rangle$, g.s. correlations induced via B

$B = 0 \;\rightarrow Y_{ph}^{\nu\,(1)}, Y_{p_1p_2h_1h_2}^{\nu\,(2)} = 0$ STDA → diagonalisation in *1p-1h + 2p-2h* model space

Stability SRPA solutions: see P. Papakonstantinou **Phys. Rev. C** 90, 024305 (2014).

Equation of Motion Phonon Method

Equation of Motion (EoM) – recursive eq. to solve **eigen-energies** on each **n**-phonon subspace while knowing the (**n-1**)-phonon eigen-energies

$$
\begin{aligned}
\mathcal{H}_0 &= \{|HF>\} \\
\mathcal{H}_1 &= \{O^\dagger_{\nu_1}|HF>\} \\
\mathcal{H}_2 &= \{O^\dagger_{\nu_1}O^\dagger_{\nu_2}|HF>\} \\
&\;\;\vdots \\
\mathcal{H}_n &= \{O^\dagger_{\nu_1}O^\dagger_{\nu_2}\ldots O^\dagger_{\nu_n}|HF>\}
\end{aligned}
$$

$$
\underbrace{< n,\beta |}_{\textbf{n}\text{-phon state}} \left\{ \left[H, O^\dagger_\lambda\right] \times \underbrace{| n-1, \alpha >}_{\textbf{(n-1)}\text{-phon state}} \right\}^\beta = \left(E^{(n)}_\beta - E^{(n-1)}_\alpha\right) \underbrace{< n,\beta |}_{\textbf{n}\text{-phon state}} \left\{ O^\dagger_\lambda \times \underbrace{| n-1, \alpha >}_{\textbf{(n-1)}\text{-phon state}} \right\}^\beta
$$

At the end we **diagonalize** nuclear **Hamiltonian** in **(0+1+2+...+n)** - phonon **basis**

$$
H = \sum_{i=1}^{A} \frac{p_i^2}{2m} + \sum_{i<j}^{A} V_{ij} = H_{int} + \frac{P^2}{2Am}
$$

Hamiltonian represented in multiphonon basis

$$
H_{intr} = \sum_{n,\alpha} E^n_\alpha |n,\alpha\rangle\langle n,\alpha| + \sum_{nn',\alpha\alpha'} |n',\alpha'\rangle\langle n',\alpha'|H_{intr}|n,\alpha\rangle\langle n,\alpha|
$$

$$
\begin{array}{c|cccc}
 & \mathcal{H}_0 & \mathcal{H}_1 & \mathcal{H}_2 & \mathcal{H}_3 \\
\hline
\mathcal{H}_0 & E_0^{(0)} & 0 & H_{02} & 0 \\
\mathcal{H}_1 & 0 & \begin{matrix} E_1^1 & & \\ & E_2^1 & \\ & & \ddots \end{matrix} & H_{12} & 0 \\
\mathcal{H}_2 & H_{20} & H_{21} & \begin{matrix} E_1^2 & & \\ & E_2^2 & \\ & & \ddots \end{matrix} & H_{23} \\
\mathcal{H}_3 & 0 & 0 & H_{32} & \begin{matrix} E_1^3 & & & \\ & E_2^3 & & \\ & & E_3^3 & \\ & & & \ddots \end{matrix}
\end{array}
$$

equiv. to STDA

Equation of Motion Phonon Method

Equation of Motion Phonon Method (**EMPM**)

$$Q_\nu^{\dagger(\mathrm{TDA})} = \sum_{ph} X_{ph}^{\nu} a_p^\dagger a_h$$

phonon excitation plays equivalent role to **1particle-1hole**

Recent applications of **EMPM**:

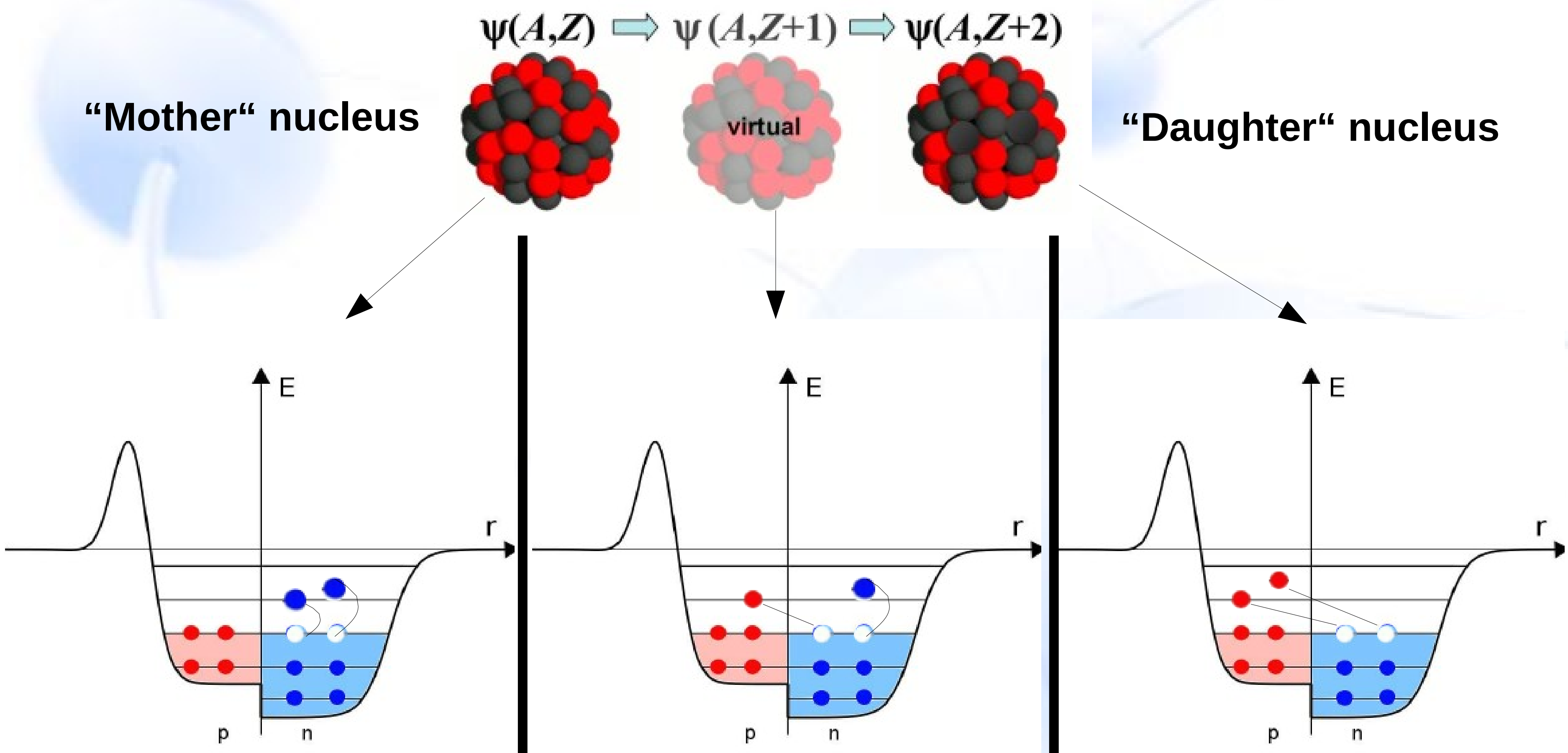
neutron-rich **closed-shell even-even** nuclei: *PRC 86 044327*; *PRC 90 014310*; *PRC 92 054315;*
neutron-rich **open-shell even-even** nuclei: *PRC 93 044314;* (**quasiparticle** formalism)
odd-even nuclei: *PRC 94 061301(R); PRC 95 034327; PRC 99 014316;*
separation of **centre-of-mass**: *PRC 105 024326; Phys. Lett. B 821 136636;*
comparison of **EMPM** to **SecondTDA** & **SecondRPA**: *PRC 107 014305;*

We demonstrated (in *PRC 107 014305*) that up-to-**2-phonon EMPM** is equivalent to **SecondTDA**. Why then just not use SecondTDA? In EMPM there is efficient method for **extracting the spurious CM** configurations (**Singular Value Decomposition Method**). EMPM at least in principle could be extended to 3-, 4- phonon calculations.

Our recent application of **Singular Value Decomposition (SVD)** Method within **EMPM** for description of spectra of ^{4}**He**, ^{8}**He**.
PRC 105 024326; Phys. Lett. B 821 136636; PRC 108 024316;

In principle, method motivated by SVD could be applied also for STDA, SRPA but not done yet.

Double Beta Decay & 2p-2h exc.



2p-2h neutron-neutron

1p-1h neutron-neutron
1p-1h proton-neutron

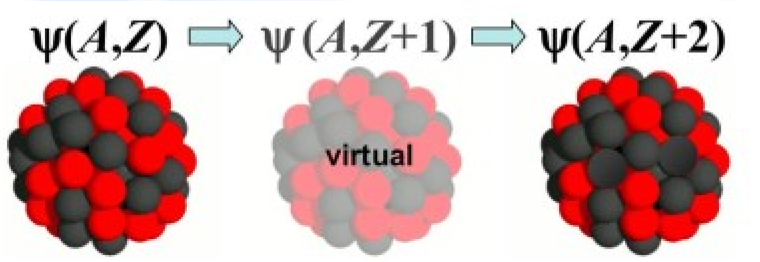
2p-2h proton-neutron

In all 3 nuclei we work with configurations up to **2particle-2hole** → we can introduce generalized **Second TDA** and/or **Second RPA** methods. Equivalently generalized **EMPM** up to 2-phonon can be formulated. Goes much further than standard (Q)RPA approaches!

Results

^{48}Ca: mean-field **s.p. energies*** taken from phenomenological Wood-Saxon
NN interaction*: **G-matrix** on **Argonne V18** potential
* obtained from F. Šimkovic

$^{48}Ca \rightarrow {}^{48}Sc$: β^- $Q_{\beta-}$ $(0^+ \rightarrow 6^+)$ = 0.2795 MeV
$^{48}Ca \rightarrow {}^{48}Ti$: $2\beta^-$ $Q_{2\beta-}$ $(0^+ \rightarrow 0^+)$ = 4.268 MeV
$T_{1/2}(^{48}Ca) = 5.6 \times 10^{19}$ years



Theor.: $Q_{\beta-}$ $(0^+ \rightarrow 6^+)$ = 1.2189 MeV
$Q_{2\beta-}$ $(0^+ \rightarrow 0^+)$ = 4.425 MeV

^{48}Ca →	^{48}Sc →	^{48}Ti	**Calc.**
|HF>	1p-1h(TDA)	2p-2h(SecTDA)	**A**
|HF>	2p-2h(SecTDA)	2p-2h(SecTDA)	**B**
|HF>+2p-2h	2p-2h(SecTDA)	2p-2h(SecTDA)	**C**

By comparison of the **A, B, C** calculations we'll see effect of 2p-2h.

2νββ:

$$T_{1/2}^{-1} = G_{2\nu} \cdot g_A^4 \cdot (m_e c^2 \cdot M_{2\nu})^2,$$

$$M_{F,GT}^{2\nu} = \sum_n \frac{\langle f \parallel \mathcal{O}_{F,GT} \parallel J_n^+ \rangle \langle J_n^+ \parallel \mathcal{O}_{F,GT} \parallel i \rangle}{E_n - (E_i + E_f)/2}$$

$g_A = 1.2701$

$$\mathcal{O}_F = \sum_{k=1}^{A} \tau_k^+, \qquad \mathcal{O}_{GT} = \sum_{k=1}^{A} \tau_k^+ \sigma_{\mathbf{k}}.$$

Calc.		$M^{2\nu}$ (MeV^{-1})	$m_e c^2 * M^{2\nu}$
A	(F)	0.00207	0.00106
A	(GT)	0.1668	0.08523
B		---	---
C		---	---
Barabash**		0.0685	0.035

****A. Barabash**, *Universe 6*, 159, (2020).

Summary & Outlook

- We discussed **double beta decay (DBD)** within **particle (neutrino)** physics. Possible exotic modes (**$0\nu\beta\beta$**) of **DBD** is important for search of physics beyond **Standard Model**.

- We discussed **double beta decay (DBD)** within **nuclear** physics. Precise theoretical calculations of **nuclear matrix elements** (**NME**) of beta transitions crucial for study of **$0\nu\beta\beta$** & **$2\nu\beta\beta$ DBD.**

- We discussed computational **nuclear structure methods** which start and/or go **beyond mean-field** approximation: Hartree-Fock (**HF**), Tamm Dancoff (**TDA**) & Second Tamm Dancoff (**STDA**), Random Phase (**RPA**) & Second Random Phase (**SRPA**), Equation of Motion Phonon Methods (**EMPM**).

- Possible application of STDA, SRPA, EMPM to calculate **NME** in **Double Beta Decay**. Preliminary results of **NME** in **^{48}Ca**.

- **Tasks to be addressed**:

  - Study effect of **2p-2h** on **NME** in **^{48}Ca**.
  - Study effective value of **g_A** in **NME**.
  - Compute NME in **^{82}Se** (particle-hole formalizm with filling approximation).

Thank you for attention!!!