Nonlinear QRPA

Adam Smetana

Institute of Experimental and Applied Physics
Czech Technical University in Prague

Mikhail Krivoruchenko
Fedor Šimkovic
Jun Terasaki

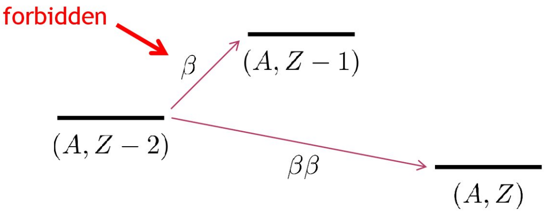
06/21/2017
Workshop INT-17-2a, Seattle

DOUBLE BETA DECAY

- nuclear matrix element must be calculated from nuclear structure model

$$\left(T_{1/2}^{\beta\beta}\right)^{-1} = g_A^4 G^{\beta\beta} |M^{\beta\beta}|^2 \left(\frac{\langle m_{\beta\beta}\rangle}{m_e}\right)^2$$

- it constitutes of a nuclear transition:

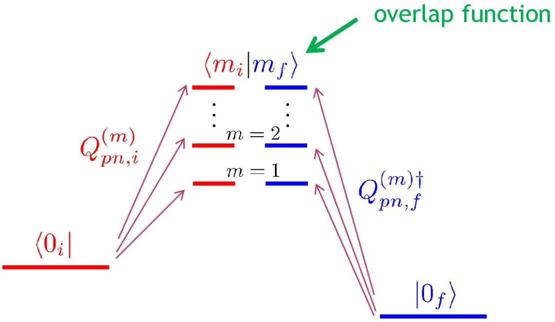


QRPA FOR DOUBLE BETA DECAY

Quasiparticle Random Phase Approximation

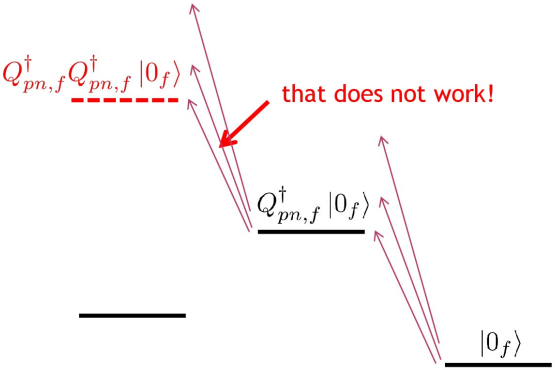
$$Q^{(m)\dagger}_{pn} = X^{(m)} A^{JM\dagger}_{pn} - Y^{(m)} \tilde{A}^{JM}_{pn}$$

$$A^{JM}_{pn} = [a_p a_n]^{JM}$$



QRPA DESCRIPTION OF MULTIPHONON STATES

- we can try to use result of the one-phonon state QRPA

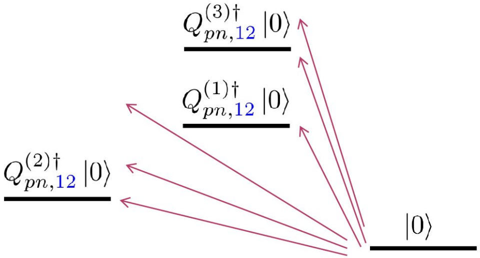


harmonic oscillator approach

it is as good approximation as well HO approximates a given hamiltonian

NONLINEAR QRPA DESCRIPTION OF MULTIPHONON STATES

- our goal is to formulate QRPA system which allows for simultaneous description of states of multiphonon origin



- for that the phonon operator must be nonlinear

$$Q^{(m)\dagger}_{pn,12} = X^{(m)} A^{JM\dagger}_{pn} - Y^{(m)} \tilde{A}^{JM}_{pn} + \ldots$$

novel approach

nonlinear phonon operators have been used to better describe the *same-nucleus* excited states

Closer look to QRPA

Derivation of QRPA starts with...

- the **Schrödinger equation**

$$H\left|n\right\rangle = E_n\left|n\right\rangle$$

- The hamiltonian is

$$H = H(A, A^\dagger, ...)$$

$$A\left|\right\rangle = 0$$

where the state $\left|\right\rangle$ is the corresponding 'unperturbed' vacuum.

Phonon operator in QRPA

...derivation of QRPA continues with...

- introducing the nth **phonon operator** $Q_n^\dagger = Q_n^\dagger(X^{(n)}, Y^{(n)})$

$$\begin{aligned} Q_n^\dagger |0\rangle &= |n\rangle \\ Q_n |0\rangle &= 0 \end{aligned}$$

which creates nth excited state $|n\rangle$ from the ground state $|0\rangle$

- This **'QRPA' equation** is fully equivalent to the Schrödinger equation

$$\langle 0| [\delta Q, H, Q_n^\dagger] |0\rangle = (E_n - E_0) \langle 0| [\delta Q, Q_n^\dagger] |0\rangle$$

where δQ is some operator.

QRPApproximation

What makes the QRPA to be an **approximation**?

1. **Truncation of the phonon operator**

$$Q_1^\dagger \equiv P_1(A, A^\dagger, \dots) \quad \longrightarrow \quad X_1 A^\dagger - Y_1 A \qquad \text{standard QRPA}$$
$$Q_n^\dagger \equiv P_n(A, A^\dagger, \dots) \quad \longrightarrow \quad Q_1^{\dagger n} \qquad \text{multiphonon approach}$$

2. **Approximation of the true ground state**

$$|0\rangle \equiv P_0(A, A^\dagger, \dots)\,|\rangle \quad \longrightarrow \quad |\mathrm{rpa}\rangle = |\rangle$$
$$\longrightarrow \quad |\mathrm{rpa}\rangle = \mathcal{N} \mathrm{e}^{dA^\dagger A^\dagger}\,|\rangle$$

3. Quasi-boson approximation ⇒ violation of Pauli Exclusion Principle (PEP)

4. Not-satisfying the ground state condition:

$$Q_n\,|\mathrm{rpa}\rangle \neq 0$$

QRPA equation

$$\langle 0| [\delta Q, H, Q_n^\dagger] |0\rangle = (E_n - E_0) \langle 0| [\delta Q, Q_n^\dagger] |0\rangle$$

Example

- phonon operator $$\begin{aligned} Q^\dagger &= XA^\dagger - YA \\ \delta Q &\in \{A^\dagger, A\} \end{aligned}$$
- RPA ground state $$|\mathrm{rpa}\rangle = |\rangle$$
- QRPA equation

$$\begin{pmatrix} \mathcal{A} & \mathcal{B} \\ \mathcal{B} & \mathcal{A} \end{pmatrix} \begin{pmatrix} X \\ Y \end{pmatrix} = (E_1 - E_0) \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} X \\ Y \end{pmatrix}$$

$$\begin{aligned} \mathcal{A} &= \langle \mathrm{rpa}| [A, H, A^\dagger] |\mathrm{rpa}\rangle \\ \mathcal{B} &= -\langle \mathrm{rpa}| [A, H, A] |\mathrm{rpa}\rangle \end{aligned}$$

Can (Q)RPA give us the exact solution?

Yes, of course!

but only for simple models

2 examples in the following
1 example by Jun Terasaki

SCHEMATIC MODEL

exactly solvable model to test quality of our approach

- ***pn*-Lipkin model** [Hirsch,Hess,Civitarese 1996]
  - it has the structure of the realistic hamiltonian
  - it is defined on a single *J*-shell with semidegeneracy Ω

$$H_F = \varepsilon C + \lambda_1 A^\dagger A + \lambda_2 (A^\dagger A^\dagger + AA)$$

where

$$C \equiv \sum_m a^\dagger_{pm} a_{pm} + \sum_m a^\dagger_{nm} a_{nm} \,, \qquad A^\dagger \equiv [a^\dagger_p a^\dagger_n]^{00}$$

  - satisfying the algebra

$$[A, A^\dagger] = 1 - C/(2\Omega) \qquad [C, A^\dagger] = 2A^\dagger$$

  - κ' parametrizes particle-particle interactions
  - χ' parametrizes particle-hole interactions

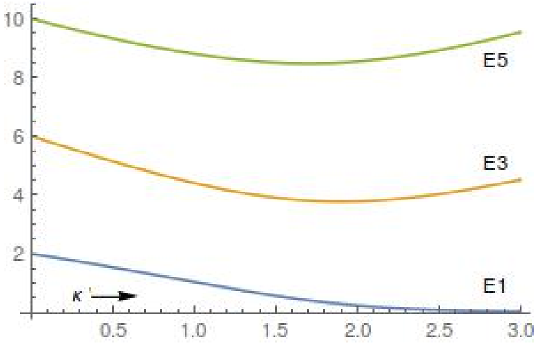
$$\begin{aligned} \lambda_1 &= 2[\chi'(u_p^2 v_n^2 + v_p^2 u_n^2) - \kappa'(u_p^2 u_n^2 + v_p^2 v_n^2)] \\ \lambda_2 &= 2(\chi' + \kappa') u_p v_p u_n v_n \end{aligned}$$

pn-Lipkin model

$$H_F = \varepsilon C + \lambda_1 A^\dagger A + \lambda_2 (A^\dagger A^\dagger + AA)$$

- decoupled systems of Ω odd and Ω even excited states
- finite number of excited states due to the Pauli exclusion principle $A^{\dagger(2\omega+1)} = 0$

$j = 3/2, \quad \Omega = 3, \quad 2 = 4, \quad N = 4, \quad \chi' = 0,$



BOSON MAPPING

Marumori mapping

$$[A, A^\dagger] = 1 - C/(2\Omega) \quad \longrightarrow \quad [B, B^\dagger] = 1$$

$$H_F \quad \longrightarrow \quad H_{BM} = \sum_{i+j \leq \max} \alpha_{ij} B^i B^{\dagger j}$$

- **bosonic model**
  - It is excellent approximation for first 2Ω eigenstates
    - already for $\max = 4$,
    - for moderate values of κ', χ', Ω,
  - up to quadratic terms
    - good approximation only for $\Omega \to \infty$

$$H_B = (2\varepsilon + \lambda_1) B^\dagger B + \lambda_2 (B^\dagger B^\dagger + BB)$$

SIMPLISTIC MODEL

*is in fact equivalent to the **Harmonic Oscillator***

$$H_B = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 q^2 + \text{const.}$$

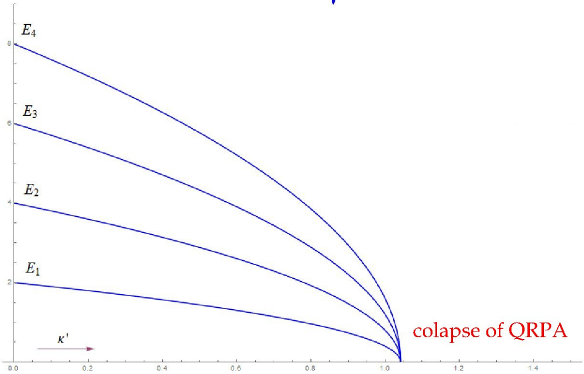
$$q = \frac{B^\dagger + B}{\sqrt{2}}, \quad p = \mathrm{i}\frac{B^\dagger - B}{\sqrt{2}}, \quad [q,p] = \mathrm{i}$$

$$\frac{1}{m} = (2\varepsilon + \lambda_1 - 2\lambda_2)$$

$$m\omega^2 = (2\varepsilon + \lambda_1 + 2\lambda_2)$$

- it has a text-book solution:

$$E_n - E_0 = nE, \quad E = \omega = \sqrt{(2\varepsilon + \lambda_1)^2 - 4\lambda_2^2}$$



STANDARD QRPA

- define a ***linear*** phonon operator

$$Q_1^\dagger = X_1 B^\dagger - Y_1 B$$

- set an Ansatz for the ground state

$$|0\rangle = \mathcal{N} \mathrm{e}^{d B^\dagger B^\dagger} \, |\rangle \; , \quad \mathcal{N}^2 = \sqrt{1 - 4d^2}$$

- annihilation condition determines the ground state parameter

$$Q_1 \, |0\rangle = 0 \implies d = \frac{1}{2} \frac{Y_1}{X_1}$$

STANDARD QRPA

RPA equation of motion

$$\begin{pmatrix} \mathcal{A}_1 & \mathcal{B}_1 \\ \mathcal{B}_1 & \mathcal{A}_1 \end{pmatrix} \begin{pmatrix} X_1 \\ Y_1 \end{pmatrix} = E \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} X_1 \\ Y_1 \end{pmatrix}$$

$$\mathcal{A}_1 = \langle 0| [B, H_B, B^\dagger] |0\rangle = 2\varepsilon + \lambda_1 \,, \quad \mathcal{B}_1 = -\langle 0| [B, H_B, B] |0\rangle = 2\lambda_2$$

- RPA eq. has an analytic solution

$$\begin{aligned} E &= \sqrt{\mathcal{A}_1^2 - \mathcal{B}_1^2} \\ X_1 &= \frac{\mathcal{A}_1 + E}{\sqrt{(\mathcal{A}_1 + E)^2 - \mathcal{B}_1^2}} \\ Y_1 &= \frac{-\mathcal{B}_1}{\sqrt{(\mathcal{A}_1 + E)^2 - \mathcal{B}_1^2}} \end{aligned}$$

$$\begin{aligned} E &= \sqrt{(2\varepsilon + \lambda_1)^2 - 4\lambda_2^2} \\ d &= -\frac{(2\varepsilon + \lambda_1) - E}{4\lambda_2} \end{aligned}$$

Exact solution reproduced!

QRPA FOR THE 2ND EXCITED STATE

- define a *nonlinear* phonon operator

$$Q_2^\dagger = X_2(B^\dagger B^\dagger + c_2) - Y_2(BB + c_2)$$

- keep the Ansatz for the ground state

$$|0\rangle = \mathcal{N} \mathrm{e}^{d_2 B^\dagger B^\dagger} |\rangle \ , \quad \mathcal{N}^2 = \sqrt{1 - 4d_2^2}$$

- RPA eq. gets little bit more complicated

$$\begin{pmatrix} \mathcal{A}_2 & \mathcal{B}_2 \\ \mathcal{B}_2 & \mathcal{A}_2 \end{pmatrix} \begin{pmatrix} X_2 \\ Y_2 \end{pmatrix} = E_2 \begin{pmatrix} \mathcal{U}_2 & 0 \\ 0 & -\mathcal{U}_2 \end{pmatrix} \begin{pmatrix} X_2 \\ Y_2 \end{pmatrix}$$

$$\mathcal{A}_2 = \langle 0| [BB, H_B, B^\dagger B^\dagger] |0\rangle \ , \quad \mathcal{B}_2 = -\langle 0| [BB, H_B, BB] |0\rangle \ , \quad \mathcal{U}_2 = \langle 0| [BB, B^\dagger B^\dagger] |0\rangle$$

- annihilation condition

$$Q_2 |0\rangle = 0 \implies d_2, \ c_2$$

QRPA FOR THE 2ND EXCITED STATE

unexpected solution

- an analytic solution is available

$$
\begin{aligned}
d_2 &= \frac{1}{2}\sqrt[2]{\frac{Y_2}{X_2}} = -\frac{(2\varepsilon + \lambda_1) - E}{4\lambda_2} \\
c_2 &= \frac{(2d_2)}{(2d_2)^2 - 1} \\
E_2 &= 2\sqrt{(2\varepsilon + \lambda_1)^2 - 4\lambda_2^2}
\end{aligned}
$$

RPA ground state and exact solution reproduced!

QRPA FOR THE 3RD EXCITED STATE

$$Q_3^\dagger = X_3(B^{\dagger 3} + c_3 B^\dagger) - Y_3(B^3 + c_3 B)$$

$$|0\rangle = \mathcal{N} \mathrm{e}^{d_3 B^\dagger B^\dagger} |\rangle$$

- follow the same procedure

$$d_3 = \frac{1}{2}\sqrt[3]{\frac{Y_3}{X_3}} = -\frac{(2\varepsilon + \lambda_1) - E}{4\lambda_2}$$

$$c_3 = \frac{3(2d_3)}{(2d_3)^2 - 1}$$

$$E_3 = 3\sqrt{(2\varepsilon + \lambda_1)^2 - 4\lambda_2^2}$$

$$d_2 = \frac{1}{2}\sqrt[2]{\frac{Y_2}{X_2}} \quad d_1 = \frac{1}{2}\frac{Y_1}{X_1}$$

$$c_2 = \frac{(2d_2)}{(2d_2)^2 - 1}$$

RPA ground state and exact solution reproduced!

QRPA FOR EVERY EXCITED STATE

A phonon operator with just two amplitudes X and Y **private** to the nth excited state

$$Q_n^\dagger = X_n \mathcal{P}_n^\dagger - Y_n \mathcal{P}_n$$

$$|\mathrm{rpa}\rangle = \mathcal{N} \mathrm{e}^{dB^\dagger B^\dagger} |\rangle$$

- where

$$\begin{aligned}
\mathcal{P}_n^\dagger &\overset{n=0}{=} 1 \\
&\overset{n=1}{=} B^\dagger \\
&\overset{n=2}{=} (B^{\dagger 2} + c) \\
&\overset{n=3}{=} (B^{\dagger 3} + 3cB^\dagger) \\
&\overset{n=4}{=} (B^{\dagger 4} + 6cB^{\dagger 2} + 3c^2) \\
&\overset{n=5}{=} (B^{\dagger 5} + 10cB^{\dagger 3} + 15c^2 B^\dagger) \\
&\overset{n=6}{=} (B^{\dagger 6} + 15cB^{\dagger 4} + 45c^2 B^{\dagger 2} + 15c^3) \\
&= \dots
\end{aligned}$$

SIMULTANEOUS DESCRIPTION FOR MORE EXCITED STATES

- (dim of RPA matrix)/2 = # of states described

- for simultaneous description of more states we need more forward and backward amplitudes
  - e.g.

$$Q^\dagger_{13} = X_3 B^{\dagger 3} + X_1 B^\dagger - Y_3 B^3 + Y_1 B$$

  - or in general

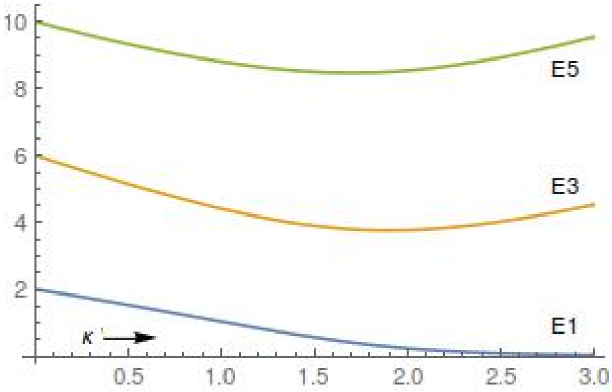
$$\boxed{Q^\dagger_{n_{\max}} = \sum_{i=1}^{n_{\max}} \left(X_i B^{\dagger i} - Y_i B^i \right)} \qquad |0\rangle = \mathcal{N} \mathrm{e}^{d B^\dagger B^\dagger} \, |\rangle$$

- it reproduces the correct spectrum of first $n_{\max}$ excited states

$$E_i = i\sqrt{(2\varepsilon + \lambda_1)^2 - 4\lambda_2^2} \quad \text{for} \quad i = 1, \ldots, n_{\max}$$

$\Omega = 3$ *pn*-Lipkin model

$$H_F = \varepsilon C + \lambda_1 A^\dagger A + \lambda_2 (A^\dagger A^\dagger + AA)$$



Exact QRPA for $\Omega = 3$ *pn*-Lipkin model

- we use full basis of operators for both Q and $|\mathrm{rpa}\rangle$:

$$Q^{\dagger}_{135} = X_1 A^{\dagger} - Y_1 A + X_3 A^{\dagger 3} - Y_3 A^3 + X_5 A^{\dagger 5} - Y_5 A^5$$
$$|\mathrm{rpa}\rangle = \left(\alpha_0 + \alpha_2 A^{\dagger 2} + \alpha_4 A^{\dagger 4} + \alpha_6 A^{\dagger 6}\right) |\rangle$$

- we satisfy the ground state condition:

$$Q_{135} |\mathrm{rpa}\rangle \stackrel{!}{=} 0 \quad \Longrightarrow \quad \alpha_{2,4,6} = f_{2,4,6}(X_1, X_3, X_5, Y_1, Y_3, Y_5)\alpha_0$$

- we does not make bosonization
- we satisfy the Pauli exclusion principle

We reproduce the exact solution!

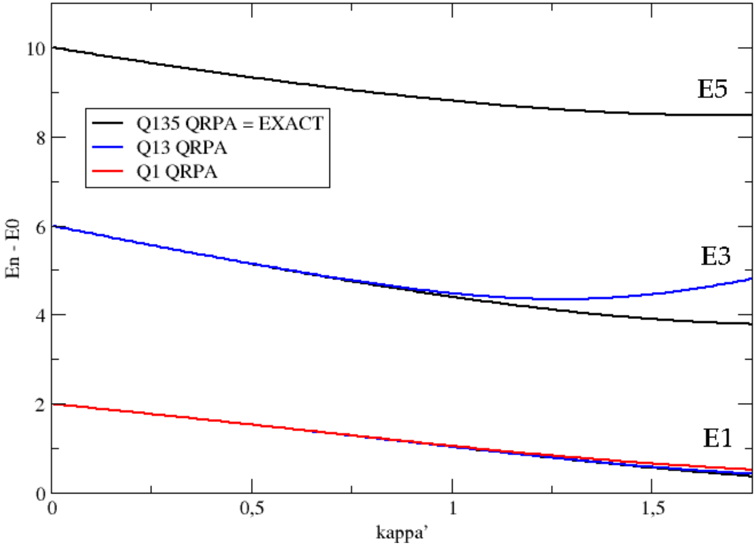
Towards realistic calculation

- **truncation of the phonon operator:**

$$
\begin{aligned}
Q^{\dagger}_{135} &= X_1 A^{\dagger} - Y_1 A + X_3 A^{\dagger 3} - Y_3 A^3 + X_5 A^{\dagger 5} - Y_5 A^5 \\
Q^{\dagger}_{13} &= X_1 A^{\dagger} - Y_1 A + X_3 A^{\dagger 3} - Y_3 A^3 \\
Q^{\dagger}_{1} &= X_1 A^{\dagger} - Y_1 A \quad \leftarrow \quad \text{PEP QRPA with } Q\,|\mathrm{rpa}\rangle = 0
\end{aligned}
$$

Energies

$j = 3/2, \quad \Omega = 3, \quad 2 = 4, \quad N = 4, \quad \chi' = 0,$

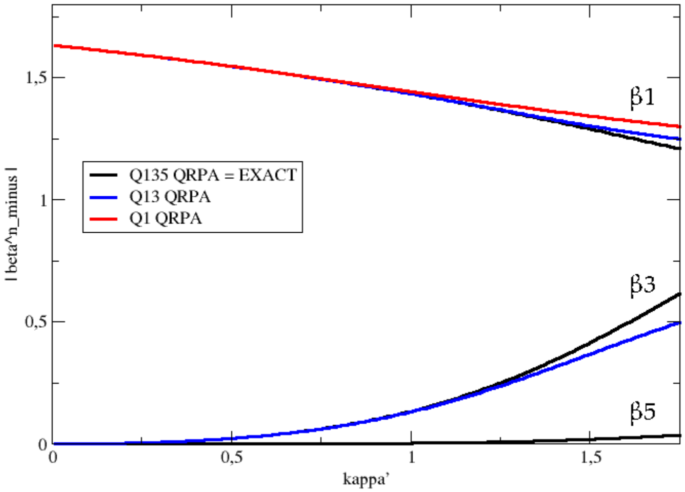


No colapse in the range of $\kappa' \sim 1.0$

Beta transitions

$$j = 3/2, \quad \Omega = 3, \quad 2 = 4, \quad N = 4, \quad \chi' = 0,$$

$$\beta_-^{(n)} = \langle \mathrm{rpa} | \, [Q^{(n)}, \beta_-] \, | \mathrm{rpa} \rangle \ , \qquad \beta_- = \sqrt{2\Omega}[u_p v_n A^\dagger + u_n v_p A]$$



Conclusions

- Quality of QRPA approach depends on choice of Q and $|\mathrm{rpa}\rangle$
- For simple models with small configuration space the exact solution from QRPA is accessible
- For realistic calculation the configuration space must be truncated or approximated for both Q and $|\mathrm{rpa}\rangle$
- We want to go beyond the truncation of the level of linear phonon operator by including non-linear terms
- We have demonstrated the improvement from the phonon operator already with the next-order nonlinearities

- Our goal is to formulate and solve the realistic QRPA system with nonlinear phonon operator relevant for $0\nu\beta\beta$
- We are now trying to understand the difficulties in numerical calculations

Towards realistic calculation

- hamiltonian

$$H = \sum_i \varepsilon_i a_i^\dagger a_i + \frac{1}{4} \sum_{ijkl} \bar{V}_{ij,kl} a_i^\dagger a_j^\dagger a_l a_k$$

- phonon operator

$$\begin{aligned} Q_k^\dagger \quad = \quad & {\color{red} c_k} + \sum_{ph} X_{ph}^k a_p^\dagger a_h + \sum_{(p_1 h_1) > (p_2 h_2)} X^k_{p_1 h_1 p_2 h_2} a_{p_1}^\dagger a_{h_1} a_{p_2}^\dagger a_{h_2} \\ & + \sum_{ph} Y_{ph}^k a_h^\dagger a_p + \sum_{(p_1 h_1) > (p_2 h_2)} Y^k_{p_1 h_1 p_2 h_2} a_{h_2}^\dagger a_{p_2} a_{h_1}^\dagger a_{p_1} \end{aligned}$$

- ground state

$$\begin{aligned} |\mathrm{rpa}\rangle \quad = \quad & \frac{1}{\mathcal{N}} \exp \Bigg[\sum_{(p_1 h_1) > (p_2 h_2)} C_{p_1 h_1 p_2 h_2} a_{p_1}^\dagger a_{h_1} a_{p_2}^\dagger a_{h_2} \\ & + \sum_{(p_1 h_1) > (p_2 h_2) > (p_3 h_3)} C_{p_1 h_1 p_2 h_2 p_3 h_3} a_{p_1}^\dagger a_{h_1} a_{p_2}^\dagger a_{h_2} a_{p_2}^\dagger a_{h_2} \Bigg] |\rangle \end{aligned}$$