Spurious states and stability condition in the extended RPA theories

V. Tselyaev

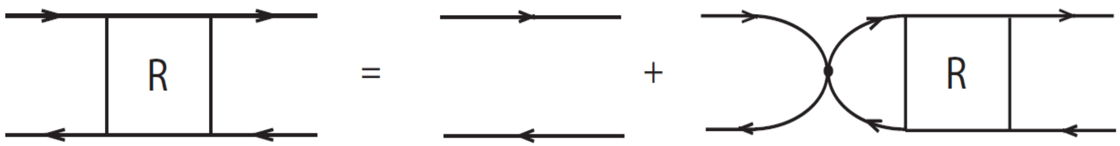
II Russian-Spanish Congress
Particle and Nuclear Physics at all Scales and Cosmology
Saint-Petersburg, October 1-4, 2013

Saint-Petersburg State University

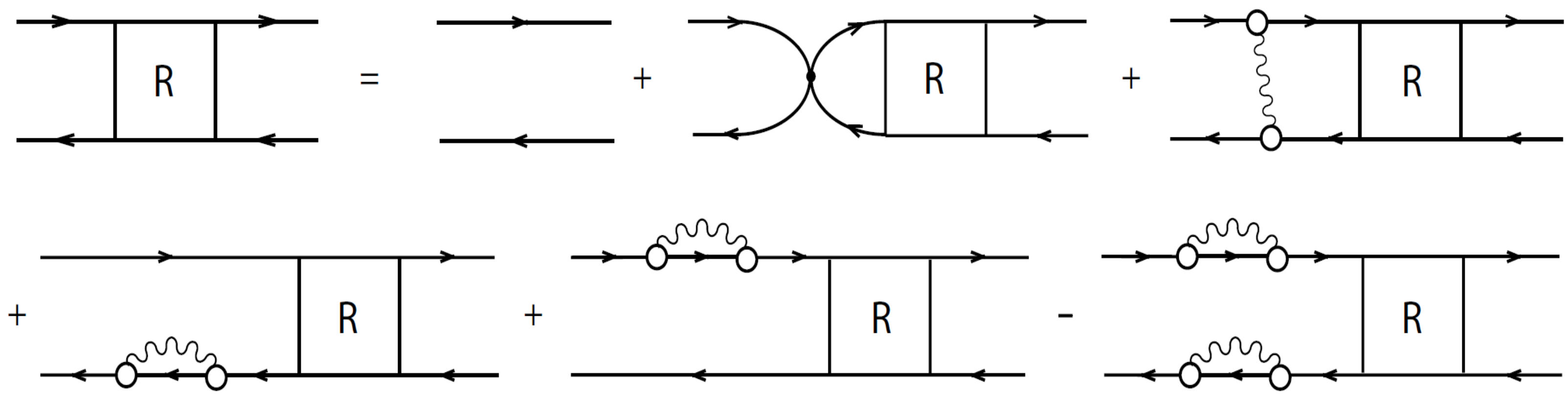
Outline

- Description of nuclear excitations within the Random Phase Approximation (RPA) and the extended RPA (ERPA) theories.
- Problem of stability and spurious states in the calculations of nuclear excitations within the ERPA.
- Stability condition in the self-consistent RPA (Thouless theorem).
- Summary of the ERPA theories.
- Dielectric theorem and subtraction method.
- Elimination of the spurious states in the ERPA.
- Stability condition in the ERPA.
- The case of a schematic model.
- Calculations of the energies of the low-lying states of ^{208}Pb within the ERPA based on the quasiparticle-phonon coupling model.
- Conclusions.

Random Phase Approximation (RPA)



Extended RPA (ERPA)



Response function formalism

$$R^{\mathrm{RPA}}(\omega) = -\left(\omega - \Omega^{\mathrm{RPA}}\right)^{-1} M^{\mathrm{RPA}}$$

$$R^{\mathrm{ERPA}}(\omega) = -\left(\omega - \Omega^{\mathrm{ERPA}}(\omega)\right)^{-1} M^{\mathrm{RPA}}$$

$$\Pi(\omega) = -\langle Q \,|\, R(\omega) \,|\, Q \rangle = \sum_n \frac{\mathrm{sgn}(\omega_n) B_n(Q)}{\omega - \omega_n}$$

Energies of the two main low-lying isoscalar 2^+ states of ^{48}Ca calculated within the RPA and the second RPA (SRPA) in a basis of 9 oscillator shells

[P. Papakonstantinou and R. Roth, Phys. Rev. C **81** (2010) 024317]
Effective interaction (UCOM) derived from the Argonne V18 potential was used.
Experimental data are taken from:
T. Hartmann, J. Enders, P. Mohr, K. Vogt, S. Volz, and A. Zilges,
Phys. Rev. C **65** (2002) 034301.

	RPA	SRPA	experiment
ω_1 (MeV)	2.19	-4.44	3.83
ω_2 (MeV)	8.12	$i \times 0.80$	8.88

RPA equations in the self-consistent theory

$$\sum_{34} \Omega^{\mathrm{RPA}}_{12,34}\, z^n_{34} = \omega_n\, z^n_{12}$$

$$\Omega^{\mathrm{RPA}}_{12,34} = h_{13}\,\delta_{42} - \delta_{13}\,h_{42} + \sum_{56} M^{\mathrm{RPA}}_{12,56}\, V_{56,34}$$

$$M^{\mathrm{RPA}}_{12,34} = \delta_{13}\,\rho_{42} - \rho_{13}\,\delta_{42}$$

$$h_{12} = \frac{\delta E[\rho]}{\delta \rho_{21}}\,, \qquad V_{12,34} = \frac{\delta^2 E[\rho]}{\delta\rho_{21}\,\delta\rho_{34}}$$

$$\rho^2 = \rho\,, \qquad [\,h, \rho\,] = 0$$

Thouless theorem in the case of the self-consistent RPA

[D. J. Thouless, Nucl. Phys. **22** (1961) 78]

$$\Omega^{\rm RPA} = M^{\rm RPA}\,\mathfrak{S}^{\rm RPA}\,, \qquad\qquad \mathfrak{S}^{\rm RPA} = M^{\rm RPA}\,\Omega^{\rm RPA}$$

$$(M^{\rm RPA})^{\dagger} = M^{\rm RPA}\,, \qquad (\mathfrak{S}^{\rm RPA})^{\dagger} = \mathfrak{S}^{\rm RPA}$$

$$\langle\, z\,|\,\mathfrak{S}^{\rm RPA}\,|\,z\,\rangle \geqslant 0\,, \quad \forall\ |\,z\,\rangle$$

$$\Longrightarrow \quad \Omega^{\rm RPA}\,|\,z^n\,\rangle = \omega_n\,|\,z^n\,\rangle\,, \qquad \omega_n^* = \omega_n$$

ERPA equations:
second RPA and the quasiparticle-phonon coupling (QPC) model within the time-blocking approximation (TBA)

$$\sum_{34} \Omega^{\mathrm{ERPA}}_{12,34}(\omega_\nu)\, z^\nu_{34} = \omega_\nu\, z^\nu_{12}$$

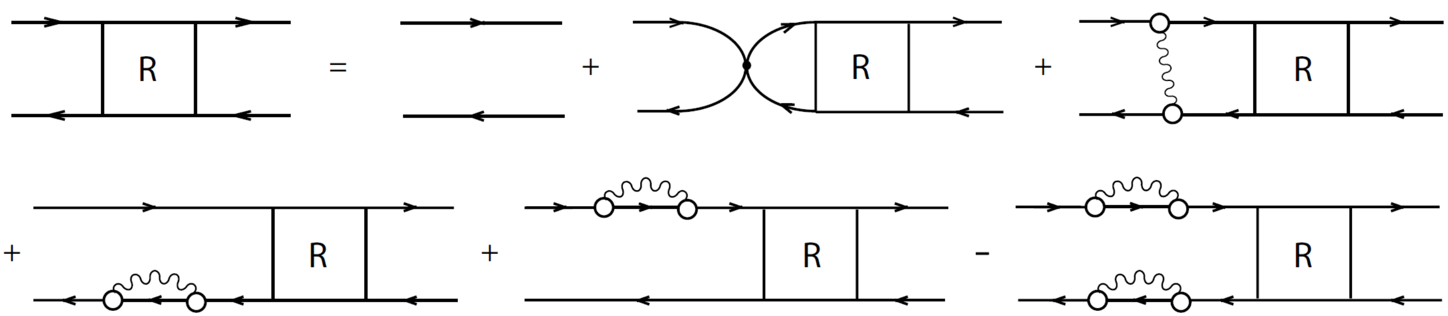
$$\Omega^{\mathrm{ERPA}}(\omega) = \Omega^{\mathrm{RPA}} + M^{\mathrm{RPA}}\, W(\omega)$$

$$W(\omega) = F(\omega - M^{\mathrm{C}}\mathfrak{S}^{\mathrm{C}})^{-1} M^{\mathrm{C}} F^{\dagger} \qquad F = \left(F^{(+)}, F^{(-)}\right)$$

$$\mathfrak{S}^{\mathrm{C}} = \begin{pmatrix} \mathfrak{S}^{\mathrm{C}(+)} & 0 \\ 0 & \mathfrak{S}^{\mathrm{C}(-)} \end{pmatrix}, \quad M^{\mathrm{C}} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$\mathfrak{S}^{\mathrm{C}(-)} = \mathfrak{S}^{\mathrm{C}(+)*}, \qquad M^{\mathrm{RPA}} F^{(\pm)} = \pm F^{(\pm)}$$

ERPA: QPC+TBA model



$$W_{12,34}(\omega) = \sum_{c,\,\sigma} \frac{\sigma\, F^{c(\sigma)}_{12}\, F^{c(\sigma)*}_{34}}{\omega - \sigma\,\Omega_c} \qquad \sigma = \pm 1$$

$$c = \{p', h', n\} \qquad \Omega_c = \varepsilon_{p'} - \varepsilon_{h'} + \omega_n\,, \quad \omega_n > 0$$

$$F^{c(-)}_{12} = F^{c(+)*}_{21} \qquad F^{c(-)}_{ph} = F^{c(+)}_{hp} = 0$$

$$F^{c(+)}_{ph} = \delta_{pp'}\, g^{n}_{h'h} - \delta_{h'h}\, g^{n}_{pp'}\,, \qquad g^{n}_{12} = \sum_{34} V_{12,34}\, z^{n}_{34}$$

Response function formalism and the dielectric theorem

[O. Bohigas, A. M. Lane, and J. Martorell, Phys. Rep. **51** (1979) 267]

$$\Pi(\omega) = -\langle Q \,|\, R(\omega) \,|\, Q \rangle = \sum_n \frac{\mathrm{sgn}(\omega_n) B_n(Q)}{\omega - \omega_n}$$

$$\Pi^{\mathrm{RPA}}(0) = -2m_{-1}^{\mathrm{RPA}} = \left(\frac{d}{d\lambda} \mathrm{Tr}\left(\rho^{(\lambda)} Q\right) \right)_{\lambda=0}$$

Density Functional Theory:

$$\mathcal{E}[\rho, \lambda] = E[\rho] + \lambda \, \mathrm{Tr}\left(\rho Q\right)$$

$$E[\rho] \sim H, \qquad \mathcal{E}[\rho, \lambda] \sim H + \lambda Q$$

H is a total Hamiltonian

Subtraction method

[for more details see: V. I. Tselyaev, arXiv: 1308.1429]

$$R^{\mathrm{RPA}}(\omega) = -\left(\omega - \Omega^{\mathrm{RPA}}\right)^{-1} M^{\mathrm{RPA}}$$

$$R^{\mathrm{ERPA}}(\omega) = -\left(\omega - \Omega^{\mathrm{ERPA}}(\omega)\right)^{-1} M^{\mathrm{RPA}}$$

$$\Pi(\omega) = -\langle\, Q \,|\, R(\omega) \,|\, Q \,\rangle$$

$$\Omega^{\mathrm{ERPA}}(0) = \Omega^{\mathrm{RPA}} \quad \Longrightarrow \quad \Pi^{\mathrm{ERPA}}(0) = \Pi^{\mathrm{RPA}}(0)$$

$$\Omega^{\mathrm{ERPA}}(\omega) = \Omega^{\mathrm{RPA}} + M^{\mathrm{RPA}}\left[\, W(\omega) - \kappa\, W(0) \,\right]$$

$$\kappa = 1$$

Spurious states in the RPA

$$R^{\mathrm{RPA}}(\omega) = -\frac{a^{(0,2)}}{\omega^2} - \frac{a^{(0,1)}}{\omega} - \sum_n{}' \frac{\mathrm{sgn}(\omega_n)\,|\,z^n\rangle\langle z^n|}{\omega - \omega_n}$$

$$\Omega^{\mathrm{RPA}} a^{(0,1)} = a^{(0,2)}, \quad \Omega^{\mathrm{RPA}} a^{(0,2)} = 0$$

$$a^{(0,1)} M^{\mathrm{RPA}}\, a^{(0,k)} = a^{(0,k)}, \qquad k = 1,2$$

$$P = 1 - a^{(0,1)} M^{\mathrm{RPA}}, \qquad P^2 = P$$

$$P\, a^{(0,k)} = 0\,,\;\; k = 1,2\,; \qquad P\,|\,z^n\rangle = |\,z^n\rangle,\;\; \omega_n \neq 0$$

Elimination of the spurious states in the ERPA

$$W^{\perp}(\omega) \;=\; P^{\dagger} W(\omega) P$$

$$\langle\, z^{n} \,|\, W^{\perp}(\omega) \,|\, z^{n'} \rangle = \langle\, z^{n} \,|\, W(\omega) \,|\, z^{n'} \rangle$$

$$W(\omega) \rightarrow W^{\perp}(\omega) \qquad (F \rightarrow P^{\dagger} F)$$

$$R^{\mathrm{ERPA}}(\omega) = R^{\mathrm{RPA}}(\omega) - R^{\mathrm{RPA}}(\omega)\, \bar{W}^{\perp}(\omega)\, R^{\mathrm{ERPA}}(\omega)$$

$$\bar{W}^{\perp}(\omega) = W^{\perp}(\omega) - W^{\perp}(0)$$

$$\bar{W}^{\perp}(\omega)\, a^{(0,k)} = a^{(0,k)}\, \bar{W}^{\perp}(\omega) = 0\,, \quad k = 1, 2$$

ERPA equation in the extended space

$$\Omega^{\mathrm{ERPA}}(\omega_\nu)\,|\,z^\nu\rangle = \omega_\nu\,|\,z^\nu\rangle$$

$$\Omega^{\mathrm{ERPA}}(\omega) = \Omega^{\mathrm{RPA}} + M^{\mathrm{RPA}}\left[\,W(\omega) - \kappa\, W(0)\,\right]$$

$$\widehat{\Omega}^{\mathrm{ERPA}} = \begin{pmatrix} \Omega^{\mathrm{RPA}(\kappa)} & M^{\mathrm{RPA}}F \\ M^{\mathrm{C}}F^\dagger & M^{\mathrm{C}}\mathfrak{S}^{\mathrm{C}} \end{pmatrix}$$

$$\Omega^{\mathrm{RPA}(\kappa)} = \Omega^{\mathrm{RPA}} + \kappa\, M^{\mathrm{RPA}}F\,(\mathfrak{S}^{\mathrm{C}})^{-1}F^\dagger$$

$$\widehat{\Omega}^{\mathrm{ERPA}}\,|\,Z^\nu\rangle = \omega_\nu\,|\,Z^\nu\rangle \qquad |\,Z^\nu\rangle = \begin{pmatrix} |\,z^\nu\rangle \\ |\,\zeta^\nu\rangle \end{pmatrix}$$

Stability condition in the ERPA

$$\widehat{\Omega}^{\mathrm{ERPA}} = M^{\mathrm{ERPA}}\,\mathfrak{S}^{\mathrm{ERPA}} \qquad \mathfrak{S}^{\mathrm{ERPA}} = M^{\mathrm{ERPA}}\,\widehat{\Omega}^{\mathrm{ERPA}}$$

$$M^{\mathrm{ERPA}} = \begin{pmatrix} M^{\mathrm{RPA}} & 0 \\ 0 & M^{\mathrm{C}} \end{pmatrix}$$

$$\langle Z\,|\,\mathfrak{S}^{\mathrm{ERPA}}|Z\,\rangle = \langle\, z\,|\,\mathfrak{S}^{\mathrm{RPA}}|\,z\,\rangle + \langle\,\zeta'|\,\mathfrak{S}^{\mathrm{C}}|\,\zeta'\,\rangle + (\kappa-1)\,\langle\,\zeta''|\,\mathfrak{S}^{\mathrm{C}}|\,\zeta''\,\rangle$$

$$|Z\,\rangle = \begin{pmatrix} |\,z\,\rangle \\ |\,\zeta\,\rangle \end{pmatrix}, \quad |\,\zeta'\,\rangle = |\,\zeta\,\rangle + |\,\zeta''\,\rangle, \quad |\,\zeta''\,\rangle = (\mathfrak{S}^{\mathrm{C}})^{-1}F^{\dagger}|\,z\,\rangle$$

$$\langle\, z\,|\,\mathfrak{S}^{\mathrm{RPA}}|\,z\,\rangle \geqslant 0\,, \;\; \forall\; |\,z\,\rangle; \qquad \langle\,\zeta\,|\,\mathfrak{S}^{\mathrm{C}}|\,\zeta\,\rangle > 0\,, \;\; \forall\; |\,\zeta\,\rangle \neq 0$$

$$\kappa \geqslant 1 \quad \Longrightarrow \quad \langle Z\,|\,\mathfrak{S}^{\mathrm{ERPA}}|Z\,\rangle \geqslant 0\,, \;\; \forall\; |Z\,\rangle$$

Subtraction method: Acceleration of the convergence

$$\bar{W}(\omega) = W(\omega) - W(0)$$

$$W(\omega) = \sum_{c,\,\sigma} \frac{\sigma\,|F^{c(\sigma)}\rangle\langle F^{c(\sigma)}|}{\omega - \sigma\,\Omega_c}$$

$$W(\omega) = -\sum_{c,\,\sigma} \frac{|F^{c(\sigma)}\rangle\langle F^{c(\sigma)}|}{\Omega_c} \sum_{m=0}^{\infty} \left(\frac{\sigma\omega}{\Omega_c}\right)^m$$

$$\bar{W}(\omega) = -\sum_{c,\,\sigma} \frac{|F^{c(\sigma)}\rangle\langle F^{c(\sigma)}|}{\Omega_c} \sum_{m=1}^{\infty} \left(\frac{\sigma\omega}{\Omega_c}\right)^m$$

The case of a schematic model: RPA

$$\Omega^{\rm RPA} = \begin{pmatrix} A & B \\ -B & -A \end{pmatrix}, \quad \mathfrak{S}^{\rm RPA} = \begin{pmatrix} A & B \\ B & A \end{pmatrix}$$

$$M^{\rm RPA} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$A = \varepsilon_p - \varepsilon_h + V_{ph,ph}\,, \quad B = V_{ph,\,hp}$$

$$\omega_{{\rm RPA}\pm} = \pm\,\omega_{\rm RPA}\,, \qquad \omega_{\rm RPA} = \sqrt{A^2 - B^2}$$

$$s_{\pm}^{\rm RPA} = A \pm |B| \qquad \Longrightarrow \qquad A \geqslant |B|$$

The case of a schematic model: ERPA

$$|\,F_{ph}^{c(+)}|^2 = |\,F_{hp}^{c(-)}|^2 = g^2, \qquad F_{ph}^{c(-)} = F_{hp}^{c(+)} = 0$$

$$\Omega^{\mathrm{ERPA}}(\omega) = \begin{pmatrix} A_\kappa + C(\omega) & B \\ -B & -A_\kappa - C(-\omega) \end{pmatrix}$$

$$A_\kappa = A + \frac{\kappa\, g^2}{\Omega_c}, \qquad C(\omega) = \frac{g^2}{\omega - \Omega_c}$$

$$\beta = B/A, \quad \gamma = g/\sqrt{A\Omega_c}, \quad \omega_c = \Omega_c/A$$

$$\bar{s}_{\pm}^{\mathrm{RPA}} = s_{\pm}^{\mathrm{RPA}}/A = 1 \pm |\beta|$$

The case of a schematic model: The ERPA eigenvalue equation

$$\det\left(\Omega^{\mathrm{ERPA}}(\omega_\nu) - \omega_\nu\right) = 0\,, \qquad \omega_\nu = \pm\,\omega_\tau\,, \quad \tau = \pm 1$$

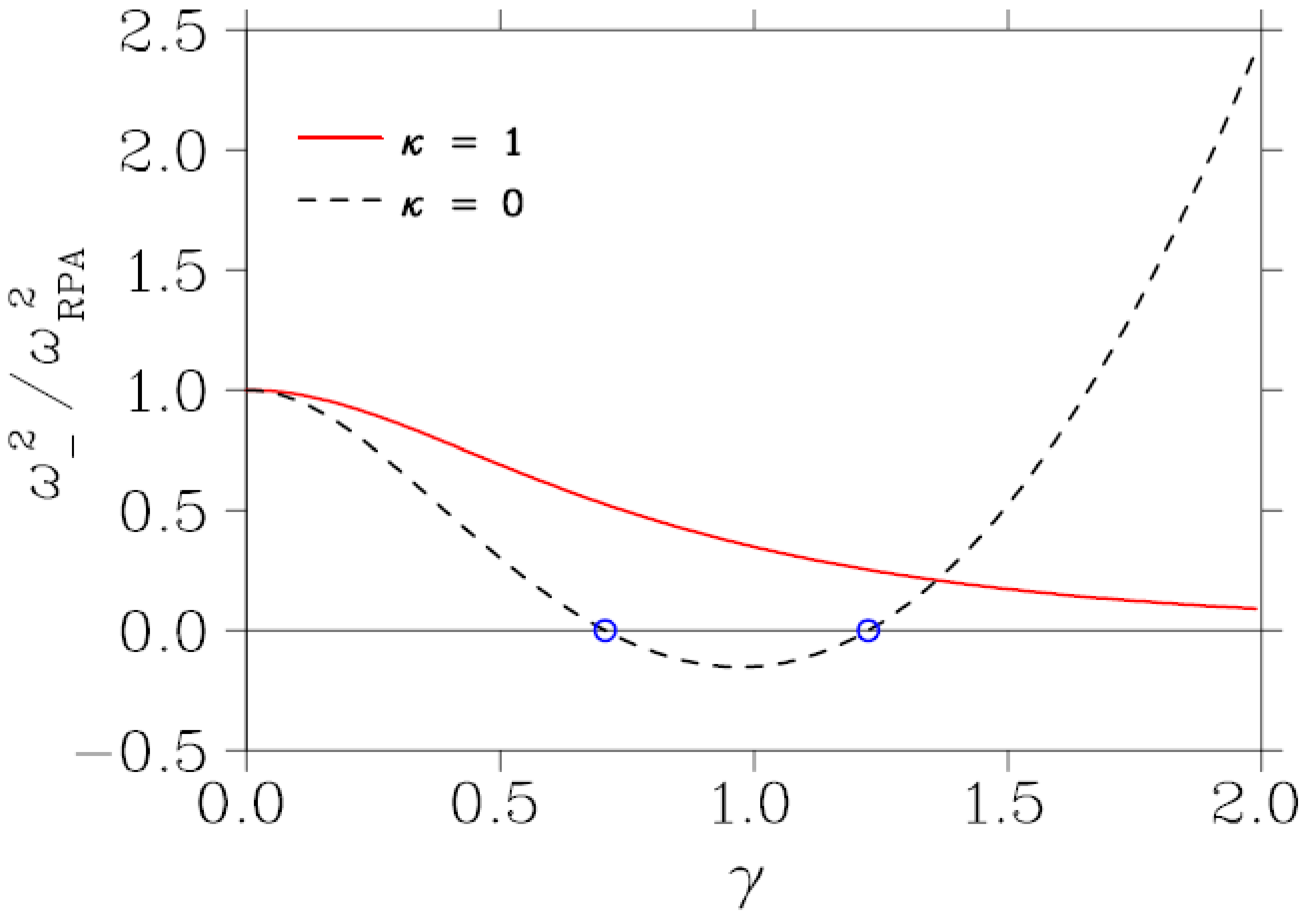
$$\omega_\tau^2 = \frac{1}{2}\left(U_\kappa^2 + \tau D_\kappa^2\right)$$

$$U_\kappa^2 = A^2\left[\,(1+\kappa\gamma^2)^2 + \omega_c^2 - \beta^2 + 2\omega_c\gamma^2\,\right]$$

$$D_\kappa^4 = U_\kappa^4 + 4A^4\omega_c^2\left(\beta^2 - [\,1 + (\kappa - 1)\,\gamma^2\,]^2\right)$$

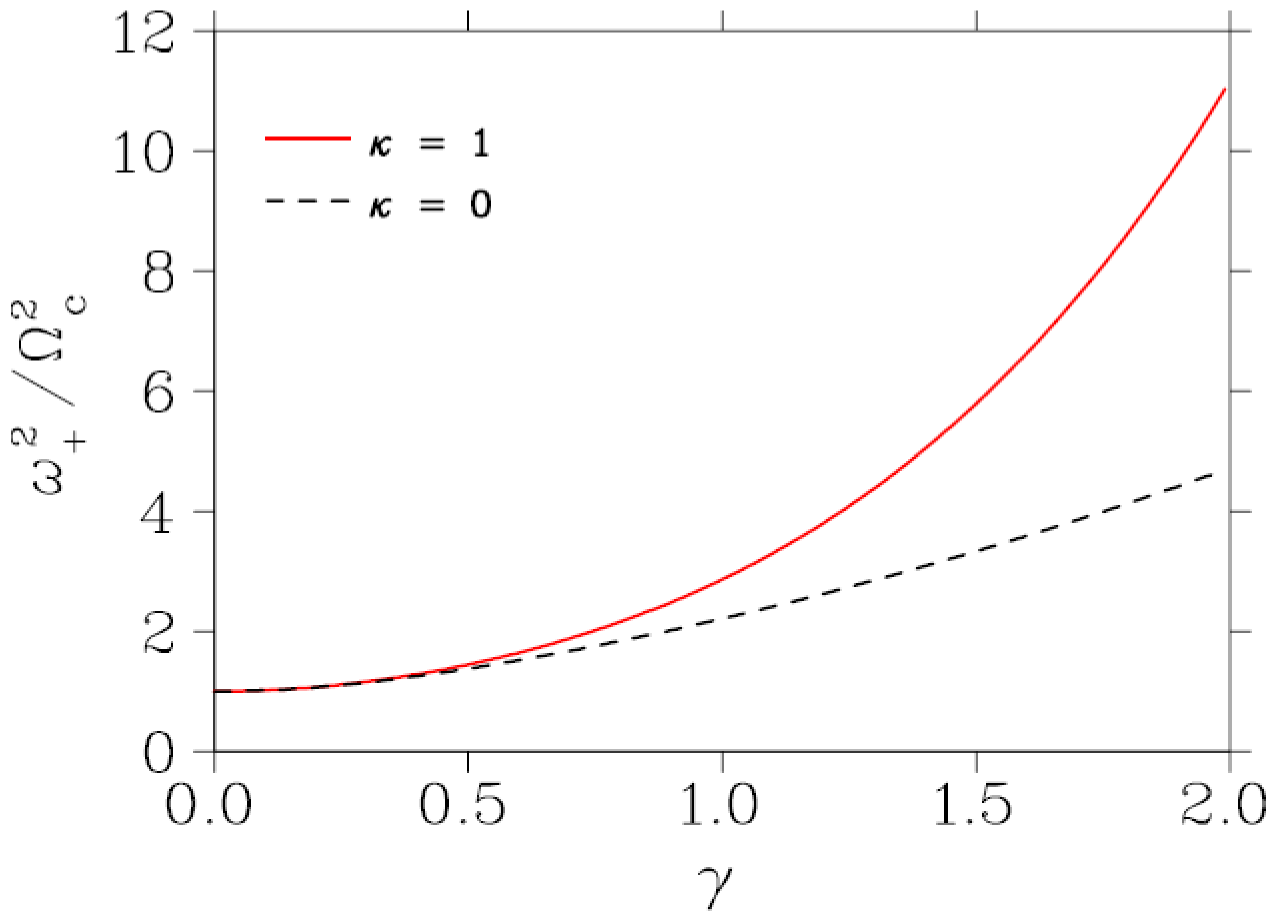
The case of a schematic model.

Dependence of the squared ERPA eigenvalue ω_{-} on the parameter γ. Calculation with $\beta = 0.5$ and $\omega_c = 2$.



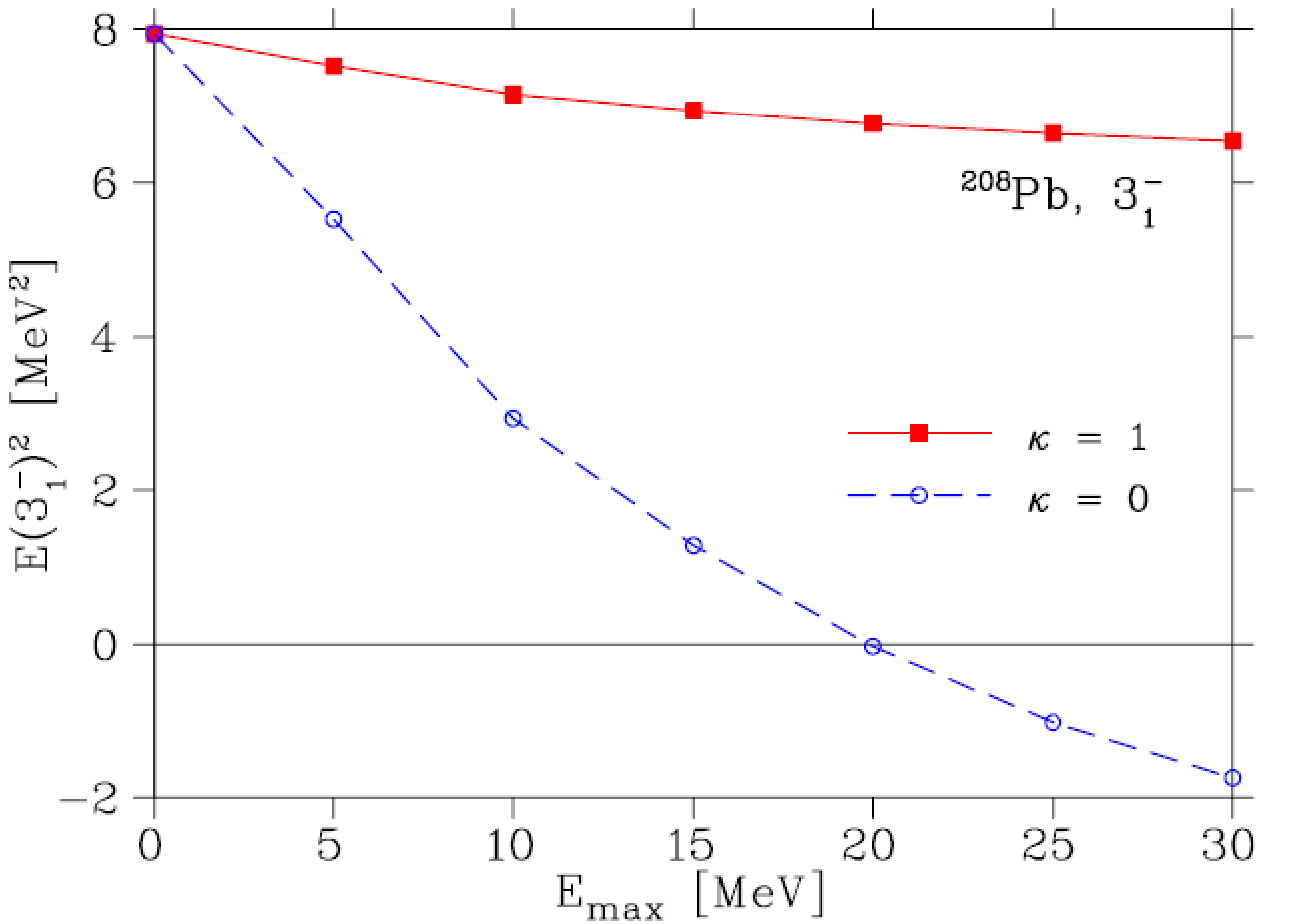
The case of a schematic model.

Dependence of the squared ERPA eigenvalue ω_+ on the parameter γ.
Calculation with $\beta = 0.5$ and $\omega_c = 2$.



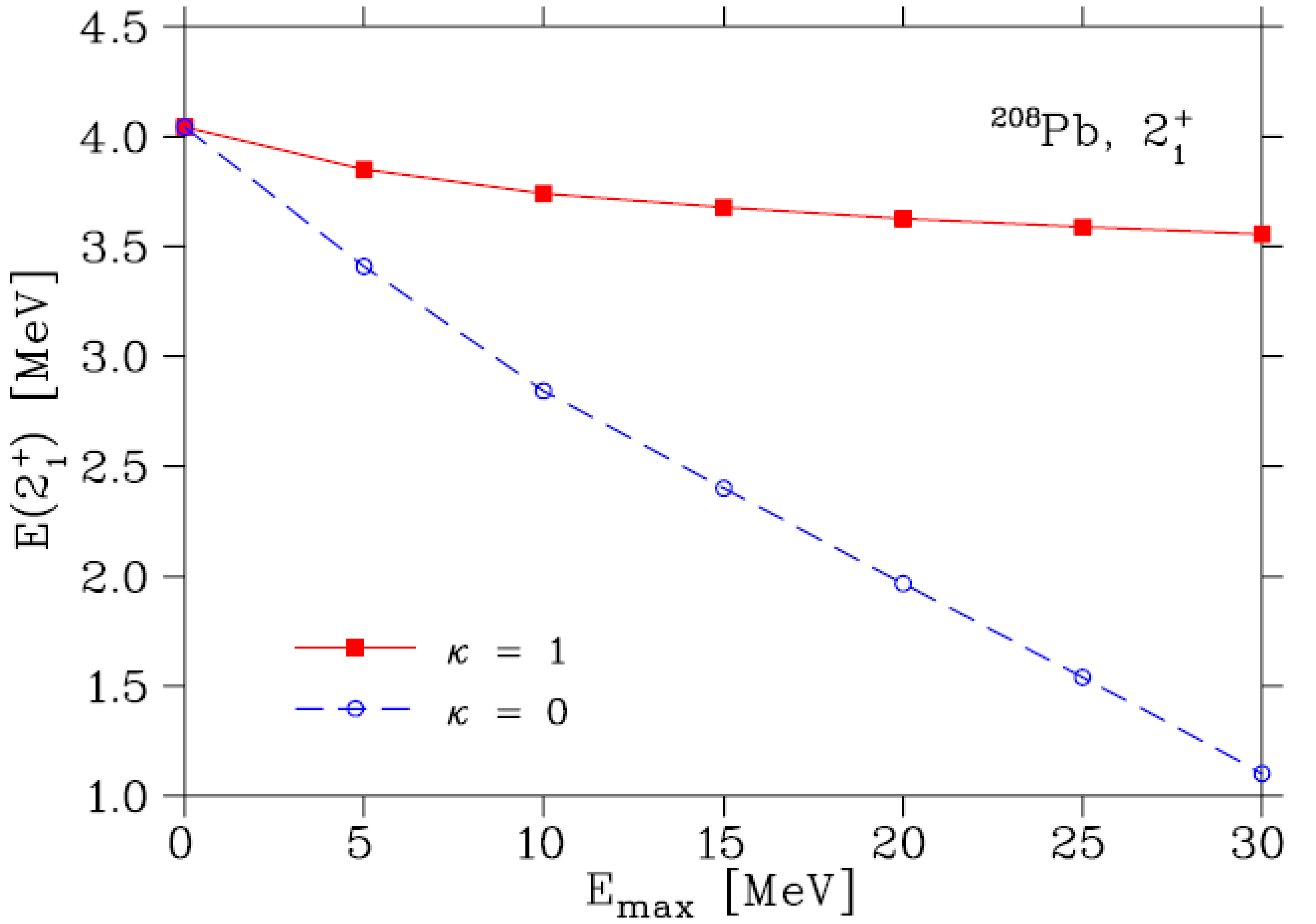
The ERPA within the QPC+TBA model.

Dependence of the squared energy of the first 3^- level in ^{208}Pb on the maximal phonon's energy of the phonon basis.
The HF mean field is calculated with the T6 Skyrme force.



The ERPA within the QPC+TBA model.

Dependence of the energy of the first 2^+ level in ^{208}Pb on the maximal phonon's energy of the phonon basis.
The HF mean field is calculated with the T6 Skyrme force.



Conclusions

- Calculations in a large model configuration space is one of the trends in the modern nuclear structure theories.
- These calculations lead to a very large downward energy shifts of the resonances in the ERPA as compared with the RPA results. In some cases, the low-lying states in the ERPA theories become unstable.
- The instability problem in the ERPA can be resolved by means of the use of the subtraction method. This method also results in the acceleration of the convergence.
- Elimination of the coupling of the spurious states to the physical modes in the ERPA is ensured by the projection technique.

Thank you!