Collective Excitations within the Second RPA

Francesco Catara[1,2], Danilo Gambacurta[1,2] and Marcella Grasso[3]

[1]Dipartimento di Fisica e Astronomia dell'Universitá di Catania

[2]Istituto Nazionale di Fisica Nucleare, Sezione di Catania

[3]Institut de Physique Nucláire - CNRS, Orsay, France

Multidisciplinary Workshop on RPA, 26-29 January 2010

Outline

RPA and SRPA

- Random Phase Approximation (RPA) and Second RPA (SRPA)
- Some properties of SRPA

Nuclear Case

- SRPA with Skyrme interaction (Density Dependent)
- The problem of the residual interaction in SRPA
- SRPA results for ^{16}O

Metallic Clusters

- SRPA in *Na* Metallic Clusters
- Extended RPA and SRPA
- Ground State Correlations are taken into account

The Method of the Equations of Motion

Set of exact eigenstates of the Hamiltonian H

$$H|\nu\rangle = E_\nu \mid \nu\rangle$$

where $\mid 0\rangle$ is the ground state with energy E_0, (H no density dependent)

Phonon Operators

Let us introduce the operators $Q's$:

$$Q_\nu^\dagger \mid 0\rangle = \mid \nu\rangle, \qquad Q_\nu \mid 0\rangle = 0.$$

Equations of Motion:

$$\langle 0 \mid \left[\delta Q, [H, Q_\nu^\dagger]\right] \mid 0\rangle = \omega_\nu \langle 0 \mid [\delta Q, Q_\nu^\dagger] \mid 0\rangle$$

where

$$\omega_\nu = E_\nu - E_0.$$

RPA and SRPA

Random Phase Approximation (RPA)

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

RPA and SRPA

Random Phase Approximation (RPA)

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

Second Random Phase Approximation (SRPA)

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

$$+ \sum_{p_1<p_2, h_1<h_2} (X_{p_1 h_1 p_2 h_2}^{(\nu)} a_{p_1}^\dagger a_{h_1} a_{p_2}^\dagger a_{h_2} - Y_{p_1 h_1 p_2 h_2}^{(\nu)} a_{h_1}^\dagger a_{p_1} a_{h_2}^\dagger a_{p_2})$$

RPA and SRPA

Random Phase Approximation (RPA)

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

Second Random Phase Approximation (SRPA)

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

$$+ \sum_{p_1<p_2, h_1<h_2} (X_{p_1 h_1 p_2 h_2}^{(\nu)} a_{p_1}^\dagger a_{h_1} a_{p_2}^\dagger a_{h_2} - Y_{p_1 h_1 p_2 h_2}^{(\nu)} a_{h_1}^\dagger a_{p_1} a_{h_2}^\dagger a_{p_2})$$

Quasi Boson Approximation (QBA)

$|\,0\rangle$ is not known: in Eqs. of Motion

$$|\,0\rangle \mapsto |\,HF\rangle$$

RPA and SRPA Equations

RPA Equations of Motion (1$\longmapsto$ 1p1h)

$$\begin{pmatrix} \mathcal{A}_{11} & \mathcal{B}_{11} \\ -\mathcal{B}^*_{11} & -\mathcal{A}^*_{11} \end{pmatrix} \begin{pmatrix} \mathcal{X}^\nu_1 \\ \mathcal{Y}^\nu_1 \end{pmatrix} = \omega_\nu \begin{pmatrix} \mathcal{X}^\nu_1 \\ \mathcal{Y}^\nu_1 \end{pmatrix}$$

RPA and SRPA Equations

RPA Equations of Motion (1$\mapsto$ 1p1h)

$$\begin{pmatrix} \mathcal{A}_{11} & \mathcal{B}_{11} \\ -\mathcal{B}^*_{11} & -\mathcal{A}^*_{11} \end{pmatrix} \begin{pmatrix} \mathcal{X}^\nu_1 \\ \mathcal{Y}^\nu_1 \end{pmatrix} = \omega_\nu \begin{pmatrix} \mathcal{X}^\nu_1 \\ \mathcal{Y}^\nu_1 \end{pmatrix}$$

SRPA Equations of Motion (1$\mapsto$ 1p1h, 2$\mapsto$ 2p2h)

$$\begin{pmatrix} \mathcal{A}_{11} & \mathcal{A}_{12} & \mathcal{B}_{11} & \mathcal{B}_{12} \\ \mathcal{A}_{21} & \mathcal{A}_{22} & \mathcal{B}_{21} & \mathcal{B}_{22} \\ -\mathcal{B}^*_{11} & -\mathcal{B}^*_{12} & -\mathcal{A}^*_{11} & -\mathcal{A}^*_{12} \\ -\mathcal{B}^*_{21} & -\mathcal{B}^*_{22} & -\mathcal{A}^*_{21} & -\mathcal{A}^*_{22} \end{pmatrix} \begin{pmatrix} \mathcal{X}^\nu_1 \\ \mathcal{X}^\nu_2 \\ \mathcal{Y}^\nu_1 \\ \mathcal{Y}^\nu_2 \end{pmatrix} = \omega_\nu \begin{pmatrix} \mathcal{X}^\nu_1 \\ \mathcal{X}^\nu_2 \\ \mathcal{Y}^\nu_1 \\ \mathcal{Y}^\nu_2 \end{pmatrix}$$

RPA and SRPA Equations

RPA Equations of Motion ($1 \mapsto$ 1p1h)

$$\begin{pmatrix} \mathcal{A}_{11} & \mathcal{B}_{11} \\ -\mathcal{B}^*_{11} & -\mathcal{A}^*_{11} \end{pmatrix} \begin{pmatrix} \mathcal{X}^\nu_1 \\ \mathcal{Y}^\nu_1 \end{pmatrix} = \omega_\nu \begin{pmatrix} \mathcal{X}^\nu_1 \\ \mathcal{Y}^\nu_1 \end{pmatrix}$$

SRPA Equations of Motion ($1 \mapsto$ 1p1h, $2 \mapsto$ 2p2h)

$$\begin{pmatrix} \mathcal{A}_{11} & \mathcal{A}_{12} & \mathcal{B}_{11} & \mathcal{B}_{12} \\ \mathcal{A}_{21} & \mathcal{A}_{22} & \mathcal{B}_{21} & \mathcal{B}_{22} \\ -\mathcal{B}^*_{11} & -\mathcal{B}^*_{12} & -\mathcal{A}^*_{11} & -\mathcal{A}^*_{12} \\ -\mathcal{B}^*_{21} & -\mathcal{B}^*_{22} & -\mathcal{A}^*_{21} & -\mathcal{A}^*_{22} \end{pmatrix} \begin{pmatrix} \mathcal{X}^\nu_1 \\ \mathcal{X}^\nu_2 \\ \mathcal{Y}^\nu_1 \\ \mathcal{Y}^\nu_2 \end{pmatrix} = \omega_\nu \begin{pmatrix} \mathcal{X}^\nu_1 \\ \mathcal{X}^\nu_2 \\ \mathcal{Y}^\nu_1 \\ \mathcal{Y}^\nu_2 \end{pmatrix}$$

QBA $|\,0\rangle \mapsto |\,HF\rangle$

$$\begin{pmatrix} \mathcal{A}_{11} & \mathcal{A}_{12} & \mathcal{B}_{11} & 0 \\ \mathcal{A}_{21} & \mathcal{A}_{22} & 0 & 0 \\ -\mathcal{B}^*_{11} & 0 & -\mathcal{A}^*_{11} & -\mathcal{A}^*_{12} \\ 0 & 0 & \mathcal{A}^*_{21} & -\mathcal{A}^*_{22} \end{pmatrix} \begin{pmatrix} \mathcal{X}^\nu_1 \\ \mathcal{X}^\nu_2 \\ \mathcal{Y}^\nu_1 \\ \mathcal{Y}^\nu_2 \end{pmatrix} = \omega_\nu \begin{pmatrix} \mathcal{X}^\nu_1 \\ \mathcal{X}^\nu_2 \\ \mathcal{Y}^\nu_1 \\ \mathcal{Y}^\nu_2 \end{pmatrix}$$

Matrices

RPA Matrices (1p1h configurations)

$$A_{1,1'} = \langle HF \mid \left[a_h^\dagger a_p, [H, a_{p'}^\dagger a_{h'}]\right] \mid HF\rangle$$

$$B_{1,1'} = -\langle HF \mid \left[a_h^\dagger a_p, [H, a_{h'}^\dagger a_{p'}]\right] \mid HF\rangle.$$

SRPA Matrices (1p1h and 2p2h configurations)

$$A_{1,2} = A_{2,1}^* = \left\langle HF\middle|\left[a_h^\dagger a_p, [H, a_{p_1}^\dagger a_{p_2}^\dagger a_{h_1} a_{h_2}]\right]\middle|HF\right\rangle$$

$$A_{2',2} = \left\langle HF\middle|\left[a_{h_2'}^\dagger a_{h_1'}^\dagger a_{p_2'} a_{p_1'}, [H, a_{p_1}^\dagger a_{p_2}^\dagger a_{h_1} a_{h_2}]\right]\middle|HF\right\rangle$$

$$B_{1,2} = B_{2,1}^* = -\left\langle HF\middle|\left[a_p^\dagger a_h, [H, a_{p_1}^\dagger a_{p_2}^\dagger a_{h_1} a_{h_2}]\right]\middle|HF\right\rangle = 0$$

$$B_{2',2} = -\left\langle HF\middle|\left[a_{p_1'}^\dagger a_{p_2'}^\dagger a_{h_1'} a_{h_2'}, [H, a_{p_1}^\dagger a_{p_2}^\dagger a_{h_1} a_{h_2}]\right]\middle|HF\right\rangle = 0$$

QBA is still used

Matrices

RPA Matrices (1p-1h configurations)

$$A_{1,1'} \sim \epsilon_{HF} + \langle ph|V|ph\rangle$$

$$B_{1,1'} \sim +\langle pp|V|hh\rangle$$

SRPA Matrices (1p-1h and 2p-2h configurations)

$$A_{1,2} \sim \langle ph|V|pp\rangle + \langle hh|V|hp\rangle$$

$$A_{2',2} \sim \epsilon_{HF} + \langle ph|V|ph\rangle + \langle pp|V|pp\rangle + \langle hh|V|hh\rangle$$

Diagonal Approximation

From SRPA to an Energy dependent RPA-like problem

- The dimension of the $\mathcal{A}_{2,2}$ matrix can be very large
- The SRPA problem can be reduced to an RPA eigenvalue problem but with $\mathcal{A}_{1,1}$ **depending on the Energy** ω

$$A_{1,1'} \mapsto \tilde{A}_{1,1'}(\omega) = A_{1,1'} + \sum_{2,2'} A_{1,2}(\omega + i\eta - A_{2,2'})^{-1} A_{2',1'}$$

- The matrix inversion is very **expensive**
- If we neglect the **residual interaction** among the $2p-2h$ states

$$A_{2,2} \simeq \delta_{h_1 h_1'} \delta_{p_1 p_1'} \delta_{h_2 h_2'} \delta_{p_2 p_2'} (\epsilon_{p_1} + \epsilon_{p_2} - \epsilon_{h_1} - \epsilon_{h_2})$$

the inversion is algebraic, (**diagonal approximation**)

Why SRPA with Skyrme?

SRPA

- SRPA should accomodate more physics than RPA
- Excitations are described in a more general way
- Coupling between $1p-1h$ and $2p-2h$ configurations (spreading width)
- Double excitations and Anharmonicities
- Low Lying States

Skyrme

- HF+RPA with Skyrme is widely and successfully used in the study of GR
- Skyrme (zero-range) interaction strongly simplify calculations
- Very useful also in SRPA
- But problem of divergence (no natural cutoff)

Skyrme interaction

$$
\begin{aligned}
V(\boldsymbol{r}_1,\boldsymbol{r}_2) = & \; t_0\,(1+x_0P_\sigma)\,\delta(\boldsymbol{r}) && \text{central term}\\
& + \frac{1}{2}t_1\,(1+x_1P_\sigma)\left[\boldsymbol{P}'^2\delta(\boldsymbol{r})+\delta(\boldsymbol{r})\boldsymbol{P}^2\right] && \\
& + t_2\,(1+x_2P_\sigma)\,\boldsymbol{P}'\cdot\delta(\boldsymbol{r})\boldsymbol{P} && \text{non-local terms}\\
& + \frac{1}{6}t_3\,(1+x_3P_\sigma)\left[\rho(\boldsymbol{R})\right]^\sigma\delta(\boldsymbol{r}) && \text{density-dependent term}\\
& + iW_0\boldsymbol{\sigma}\cdot\left[\boldsymbol{P}'\times\delta(\boldsymbol{r})\boldsymbol{P}\right] && \text{spin–orbit term}\,.
\end{aligned}
$$

with:

$$\boldsymbol{r}=\boldsymbol{r}_1-\boldsymbol{r}_2\,, \qquad \boldsymbol{R}=\frac{1}{2}(\boldsymbol{r}_1+\boldsymbol{r}_2)\,,$$

$$\boldsymbol{P}=\frac{1}{2i}(\boldsymbol{\nabla}_1-\boldsymbol{\nabla}_2)\,, \qquad \boldsymbol{P}' \text{ cc of } \boldsymbol{P} \text{ acting on the left}$$

and

$$\boldsymbol{\sigma}=\boldsymbol{\sigma}_1+\boldsymbol{\sigma}_2\,, \qquad P_\sigma=(1+\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2)/2\,.$$

SRPA with Density Dependent Force

Density Dependent Force (DDF)

- In the case of DDF, RPA equations can be derived by using the Small Amplitude Limit of Time Dependent Hartree Fock
- The residual interaction is defined as the second derivative of the energy functional
- The so called Rearrangement terms come out
- SRPA equations have never been derived in the case of DDF
- What about the Rearrangement terms in SRPA?

Main (Preliminary) Results

- Rearrangement Terms are present also in matrix elements beyond RPA
- These Rearrangement Terms have a **different expression** from the ones of the RPA matrices
- The B_{12}, B_{21} and B_{22} matrices are not zero anymore since Rearrangement Terms appear in them

Calculations for ^{16}O

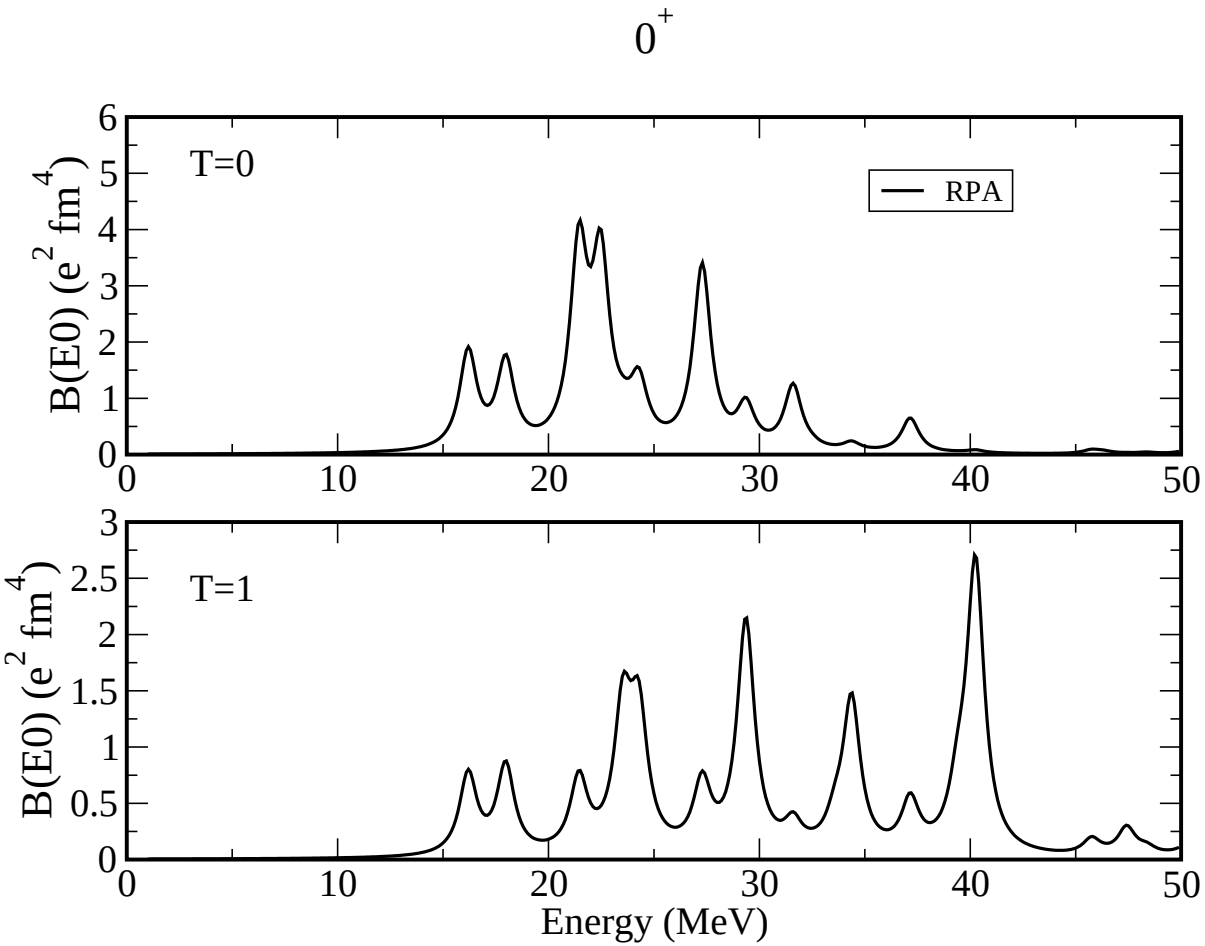
Calculations Details

- As a first step, we have solved the HF $\Rightarrow$ RPA and SRPA
- We use the Skyrme interaction (SGII)
- Monopole and Quadrupole Strength Distributions for $F_\lambda^{IS}(\mathbf{r}) = \sum r_i^2 Y_{\lambda 0}(\hat{r}_i)$ and $F_\lambda^{IV}(\mathbf{r}) = \sum r_i^2 Y_{\lambda 0}(\hat{r}_i)\tau_z(i)$
- Transition Densities

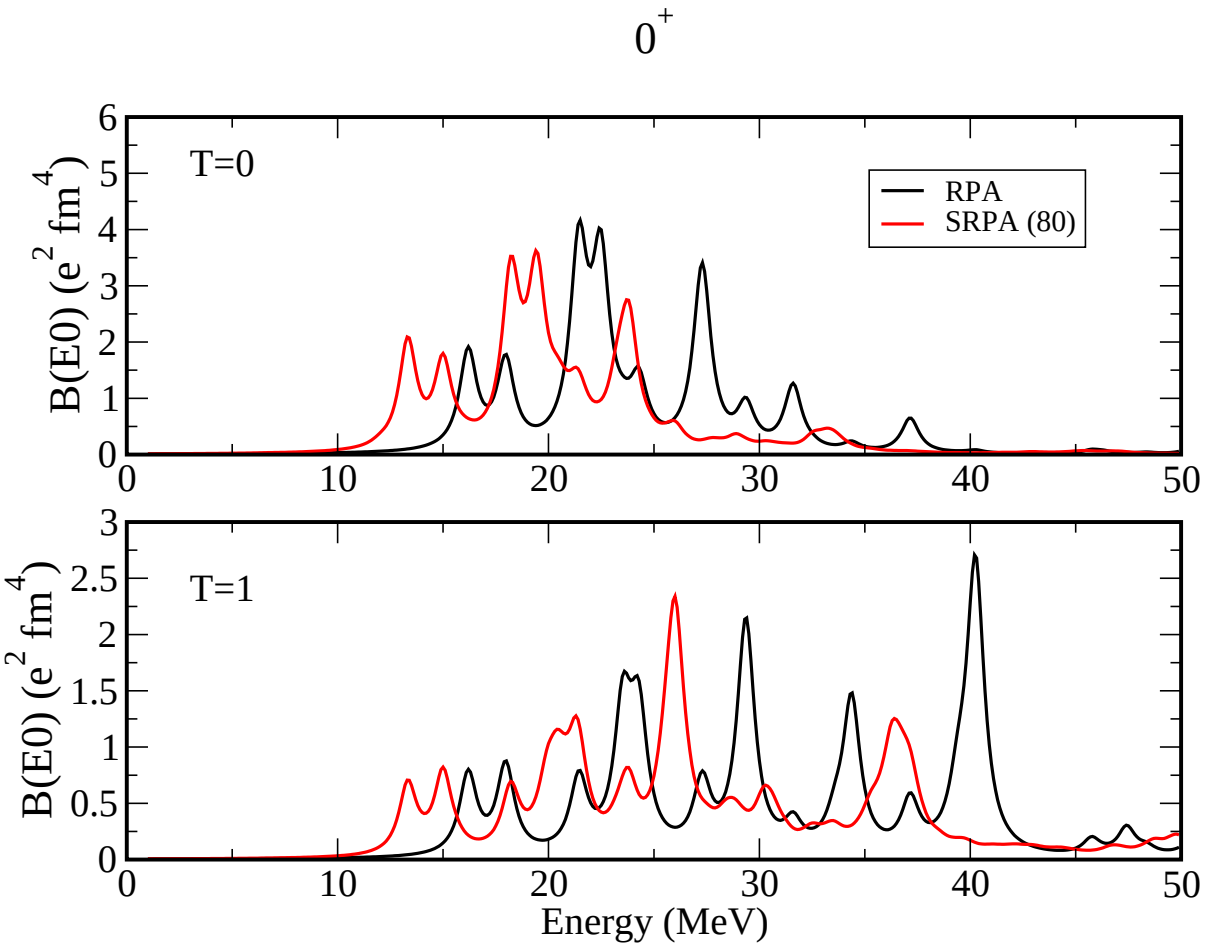
Comparison between different results

- RPA
- Full SRPA: **all kinds of couplings** among all 1p1h and 2p2h configurations
- Diagonal Approximation
- SRPA without Rearrangement Terms
- SRPA with Rearrangement Terms as defined in RPA

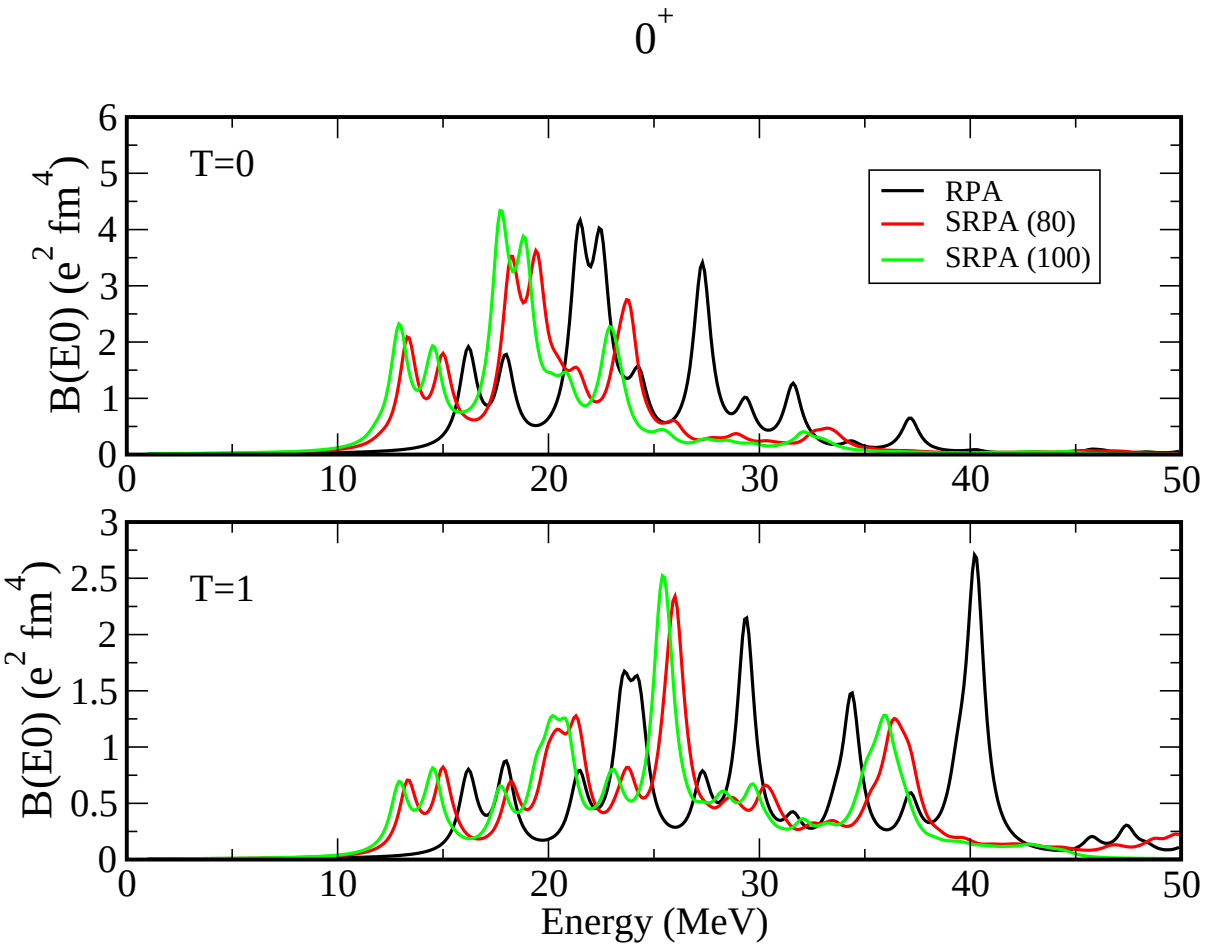
Monopole Strength Distribution, Without Rearrangement Terms



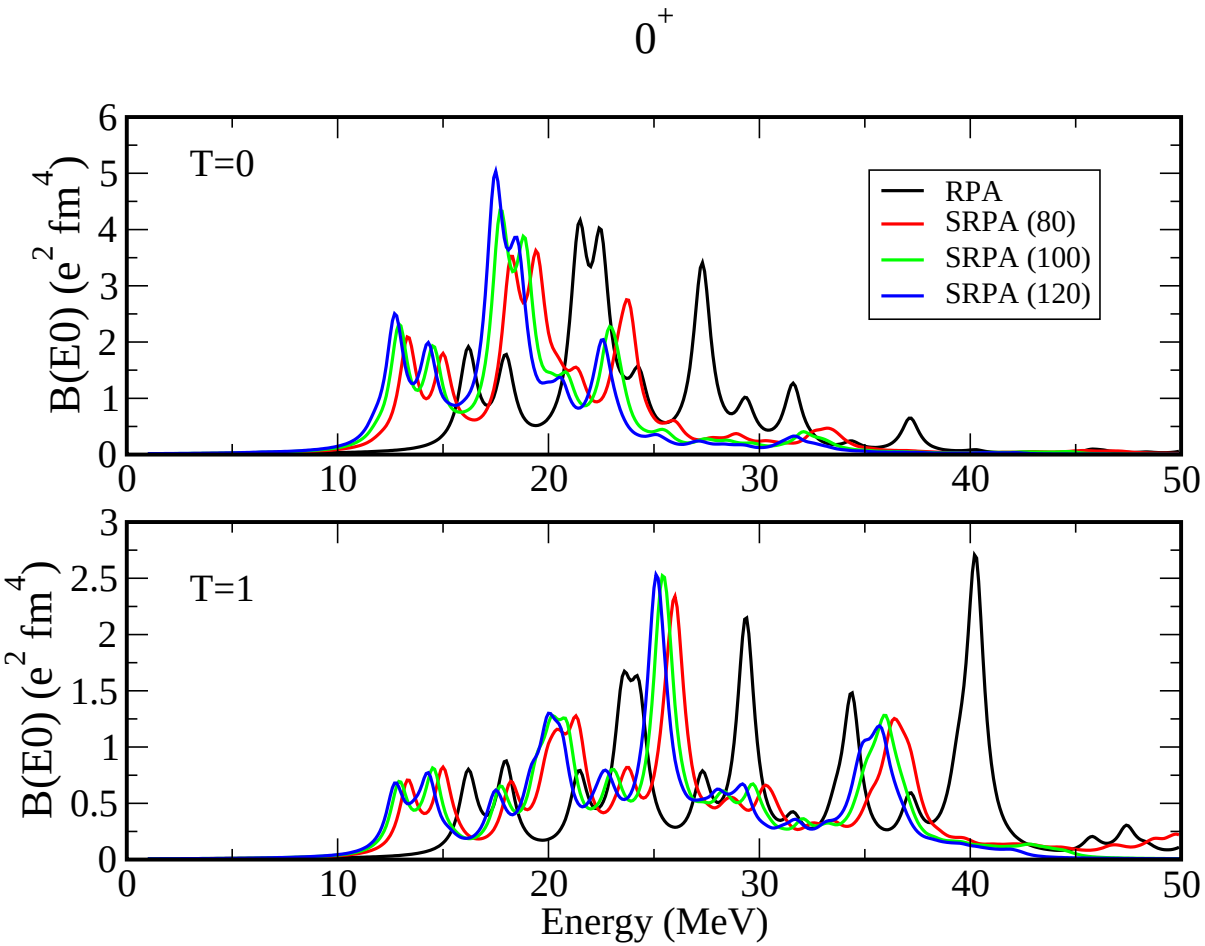
Monopole Strength Distribution, Without Rearrangement Terms



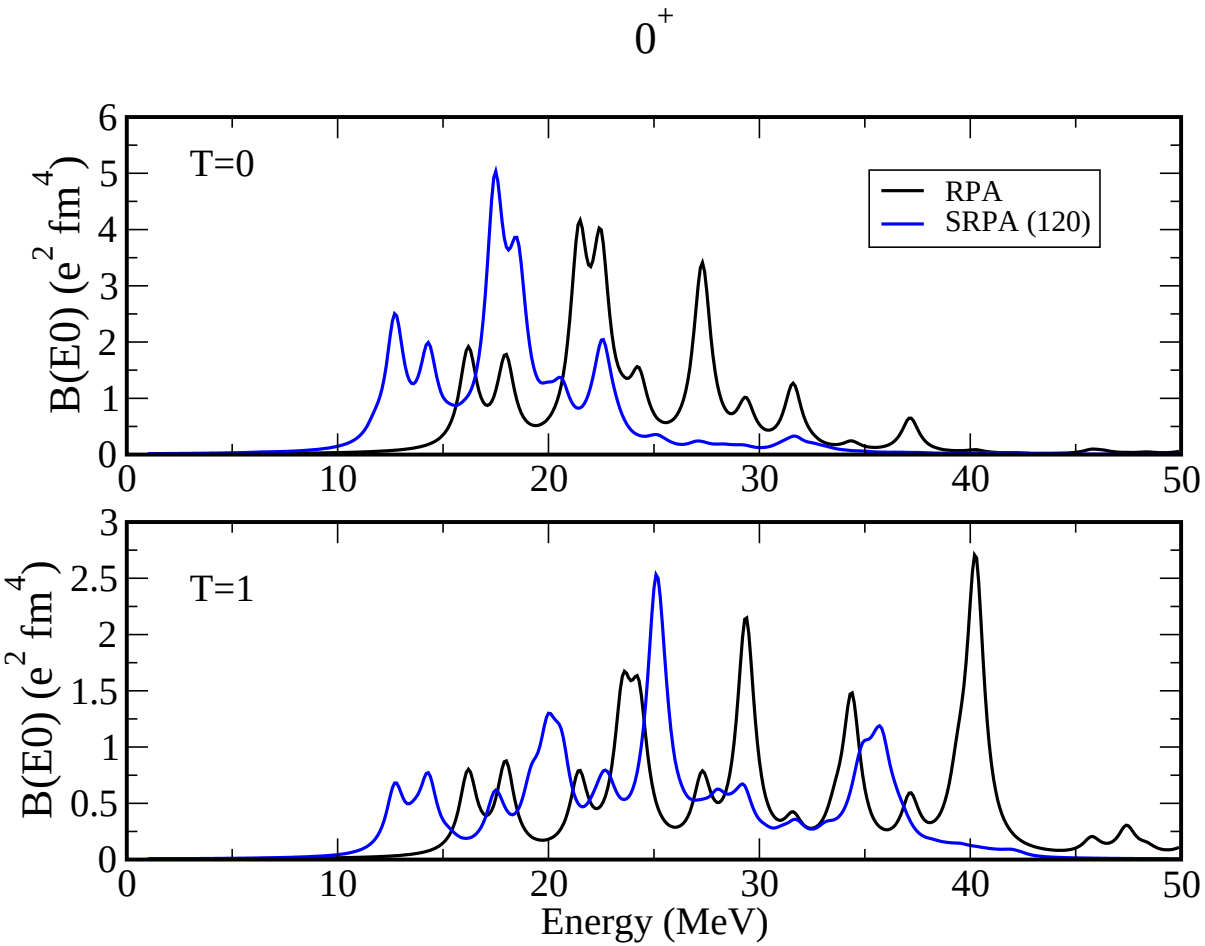
Monopole Strength Distribution, Without Rearrangement Terms



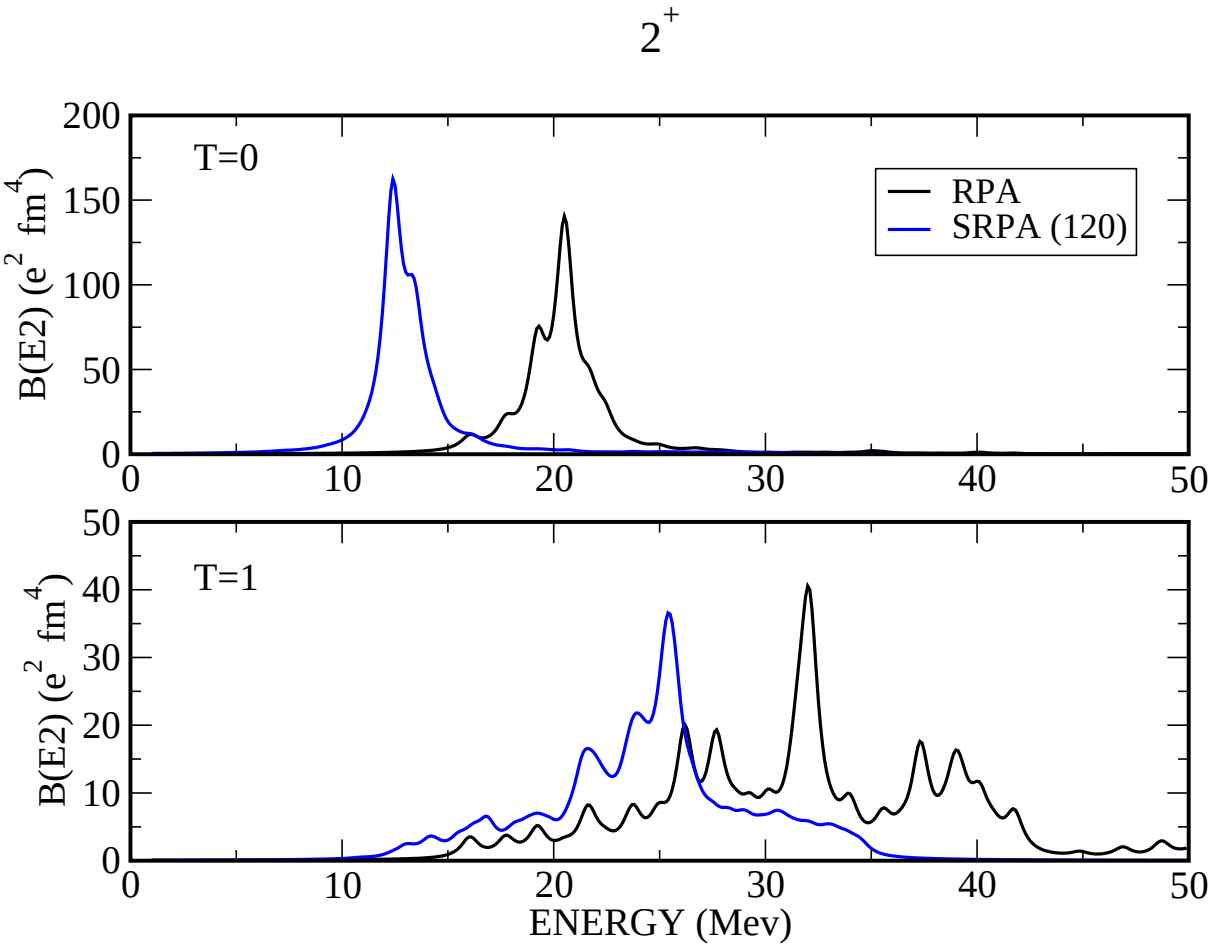
Monopole Strength Distribution, Without Rearrangement Terms



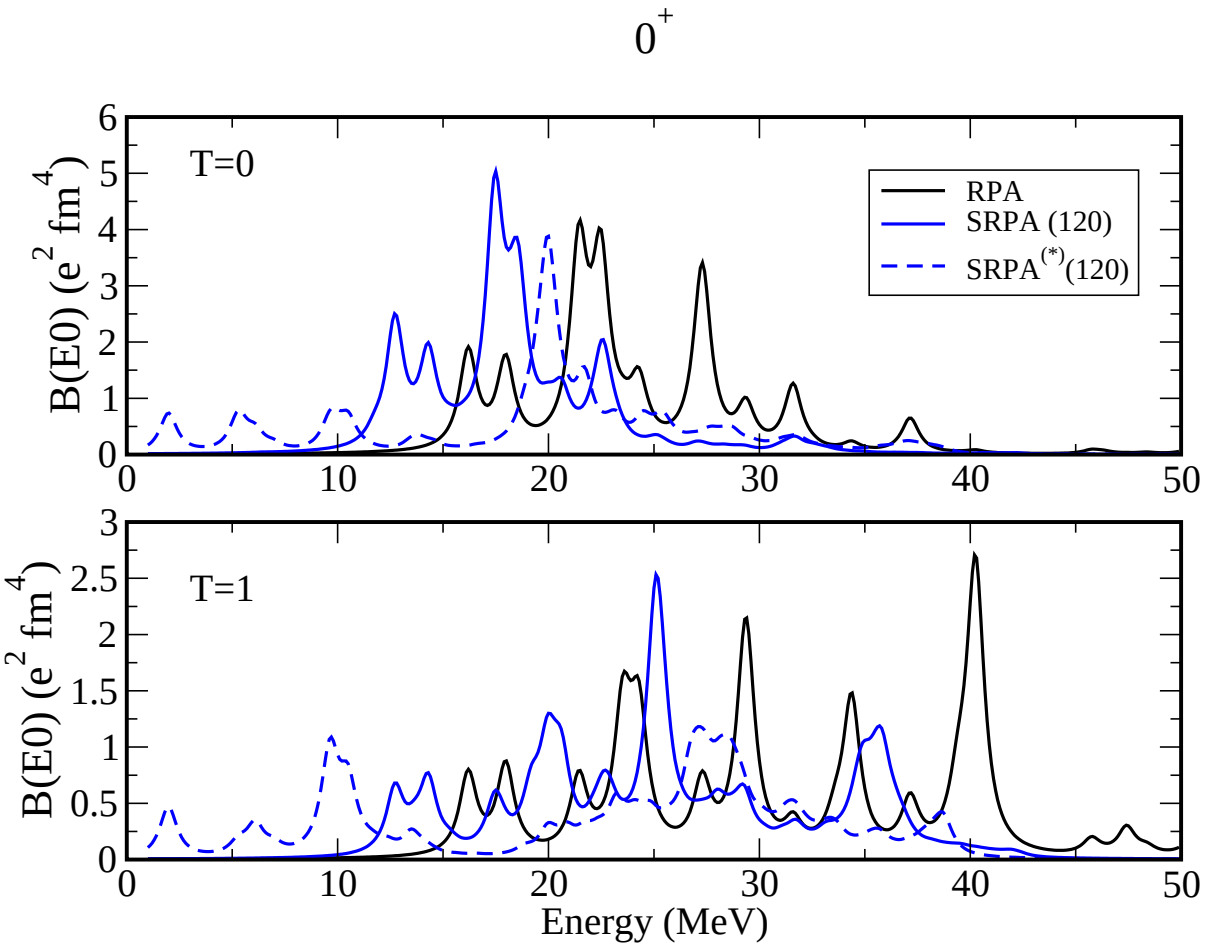
Monopole Strength Distribution, Without Rearrangement Terms



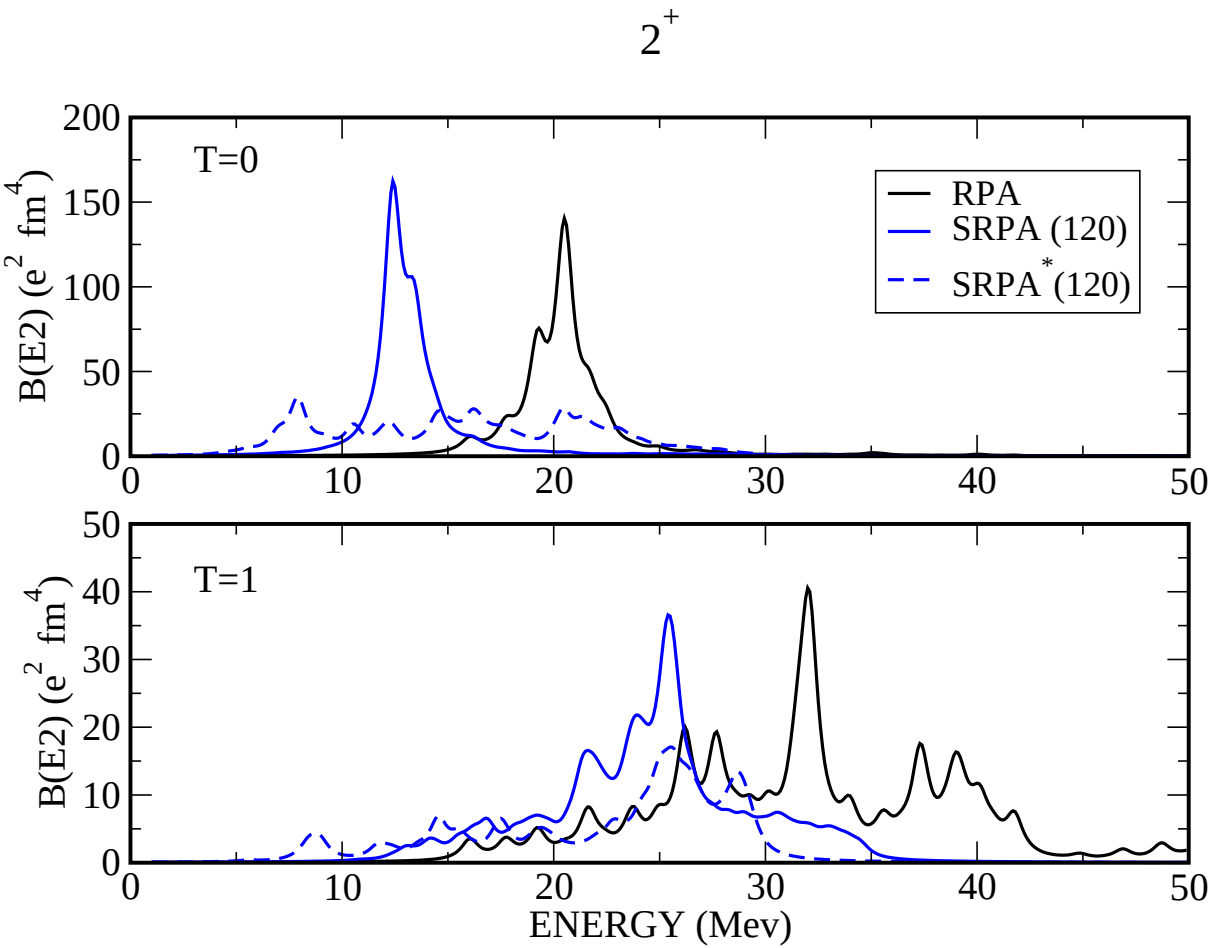
Quadrupole Strength Distribution, Without Rearrangement Terms



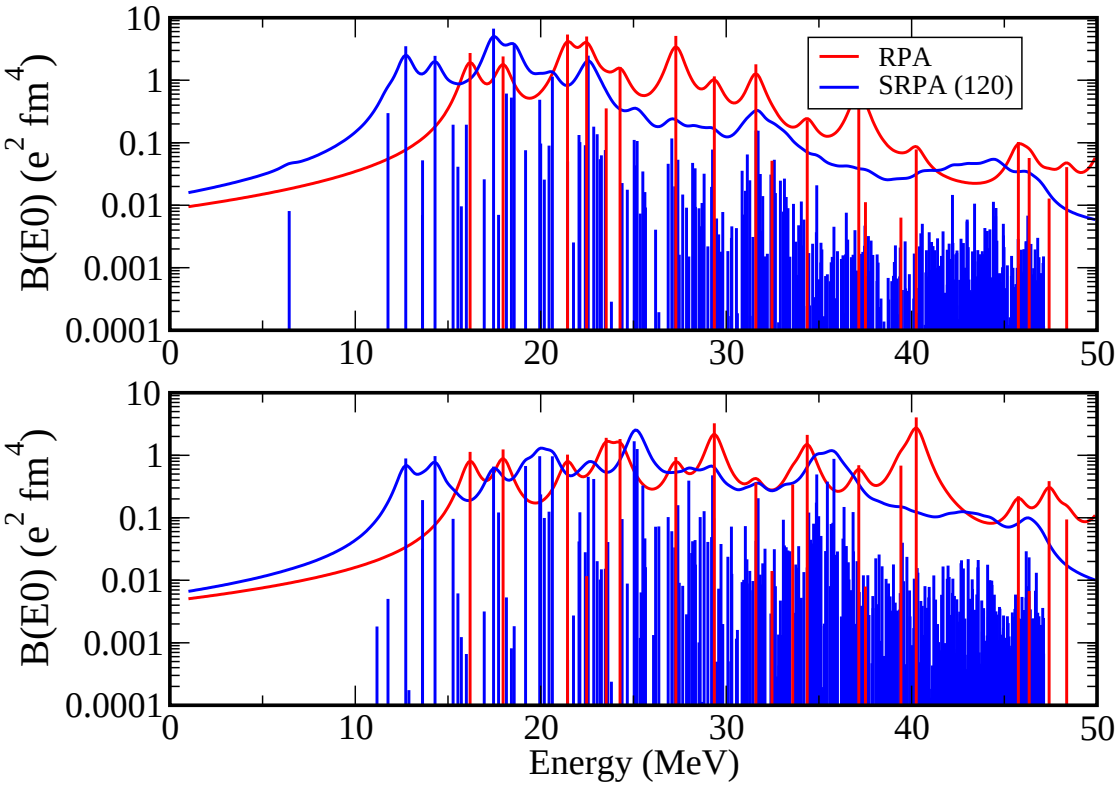
Monopole, With (SRPA*) and Without (SRPA) Rearrangement Terms



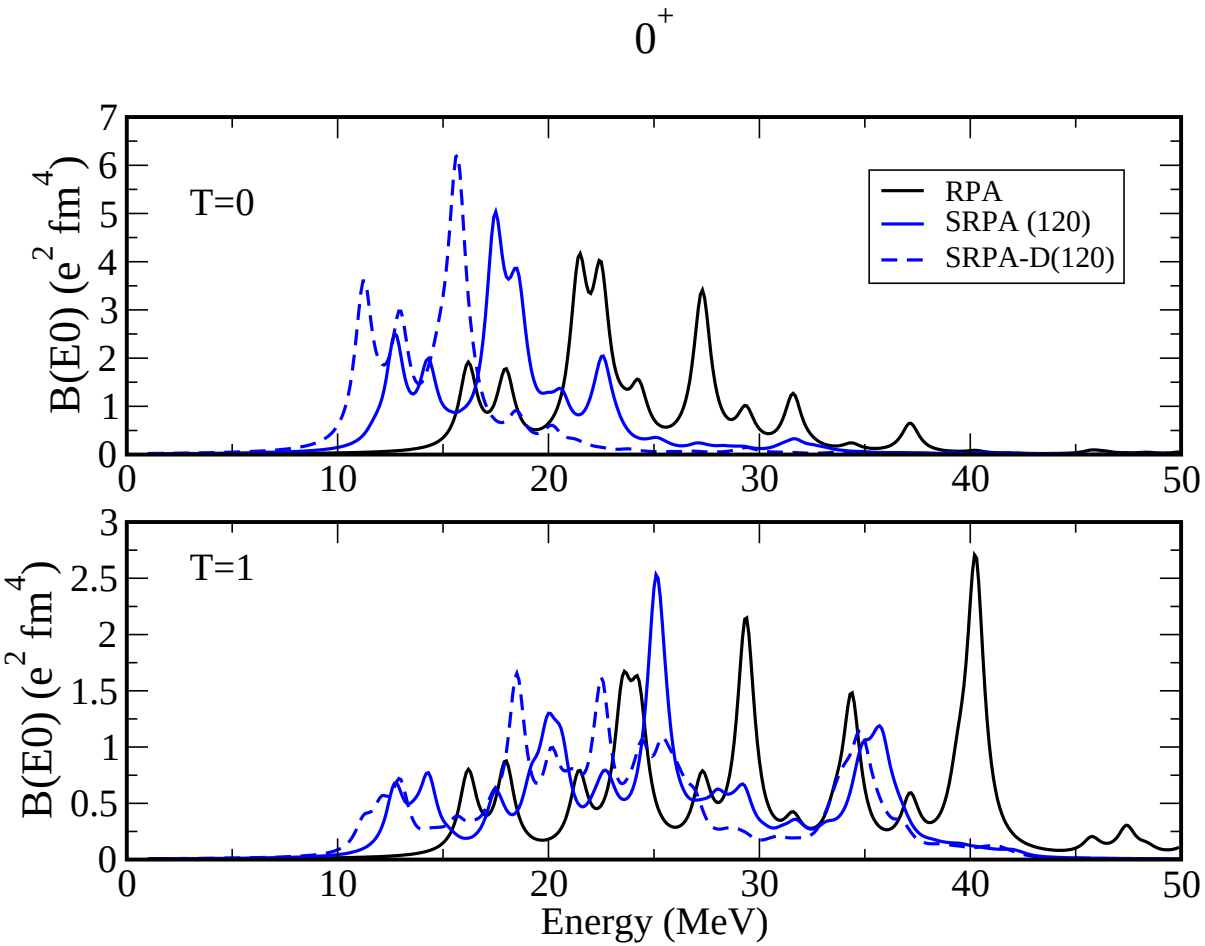
Quadrupole, With (SRPA*) and Without (SRPA) Rearrangement Terms



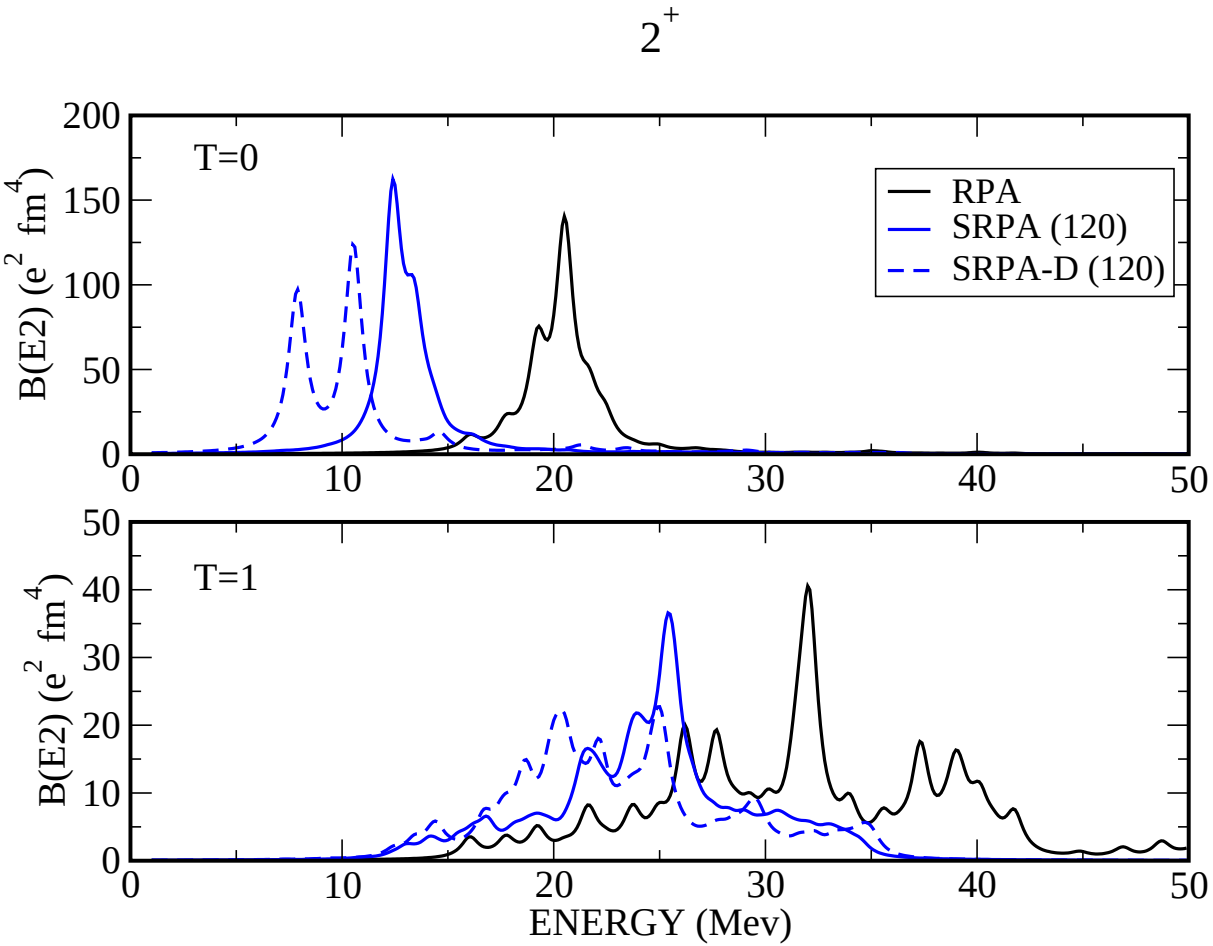
Monopole Strength Distribution, Without Rearrangement Terms



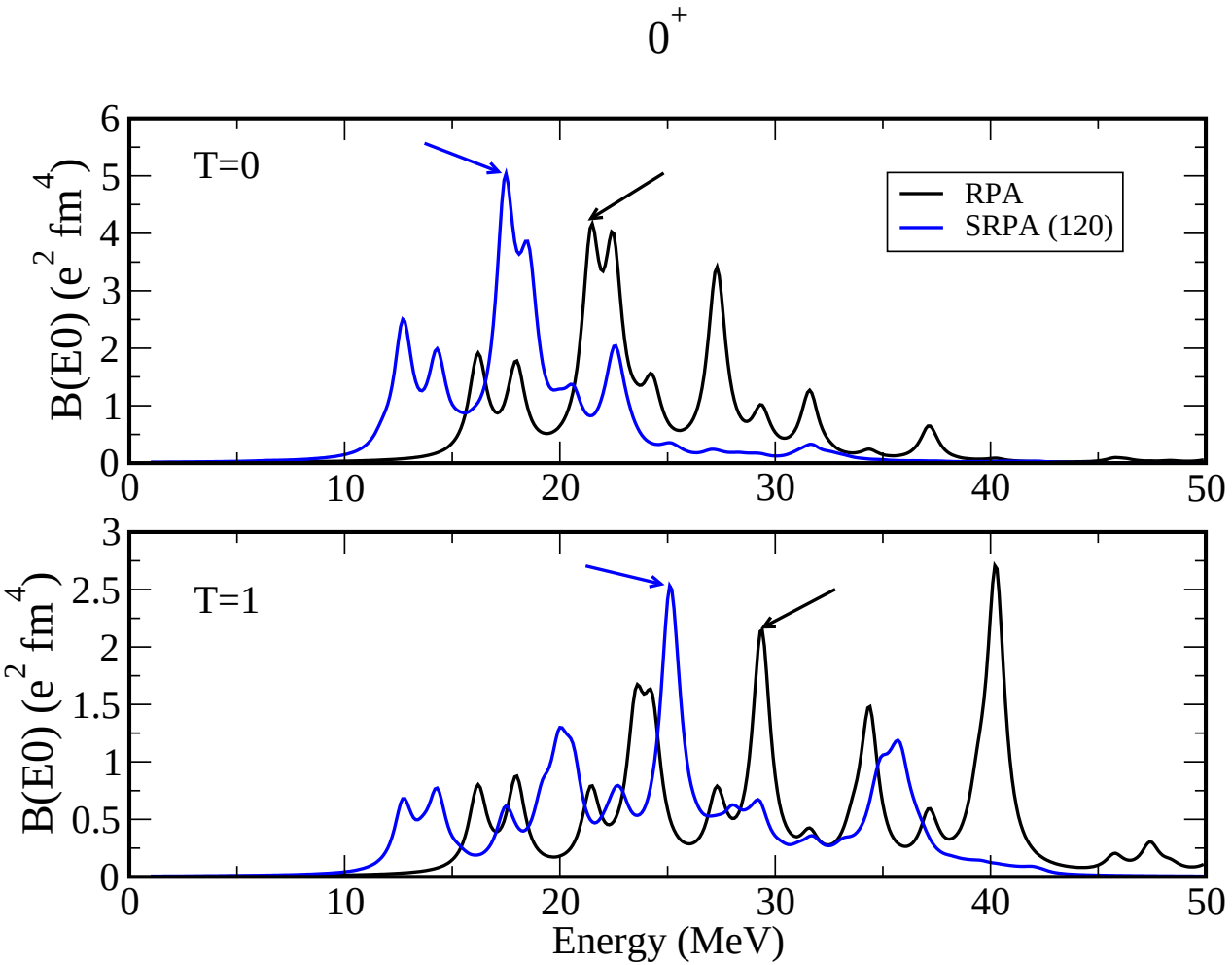
Monopole Strength, Full Vs Diagonal (No Rearrangement)



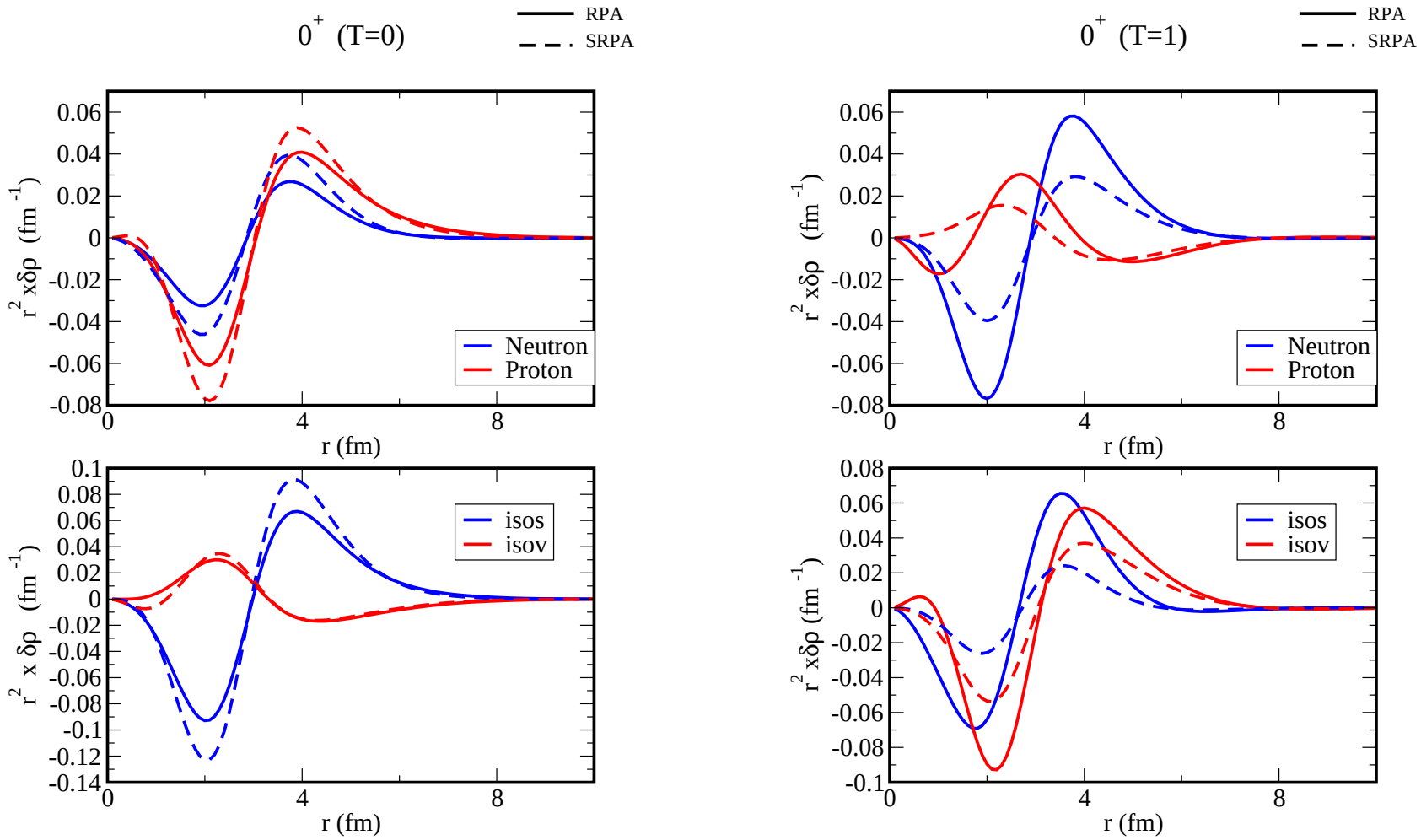
Quadrupole Strength, Full Vs Diagonal (No Rearrangement)



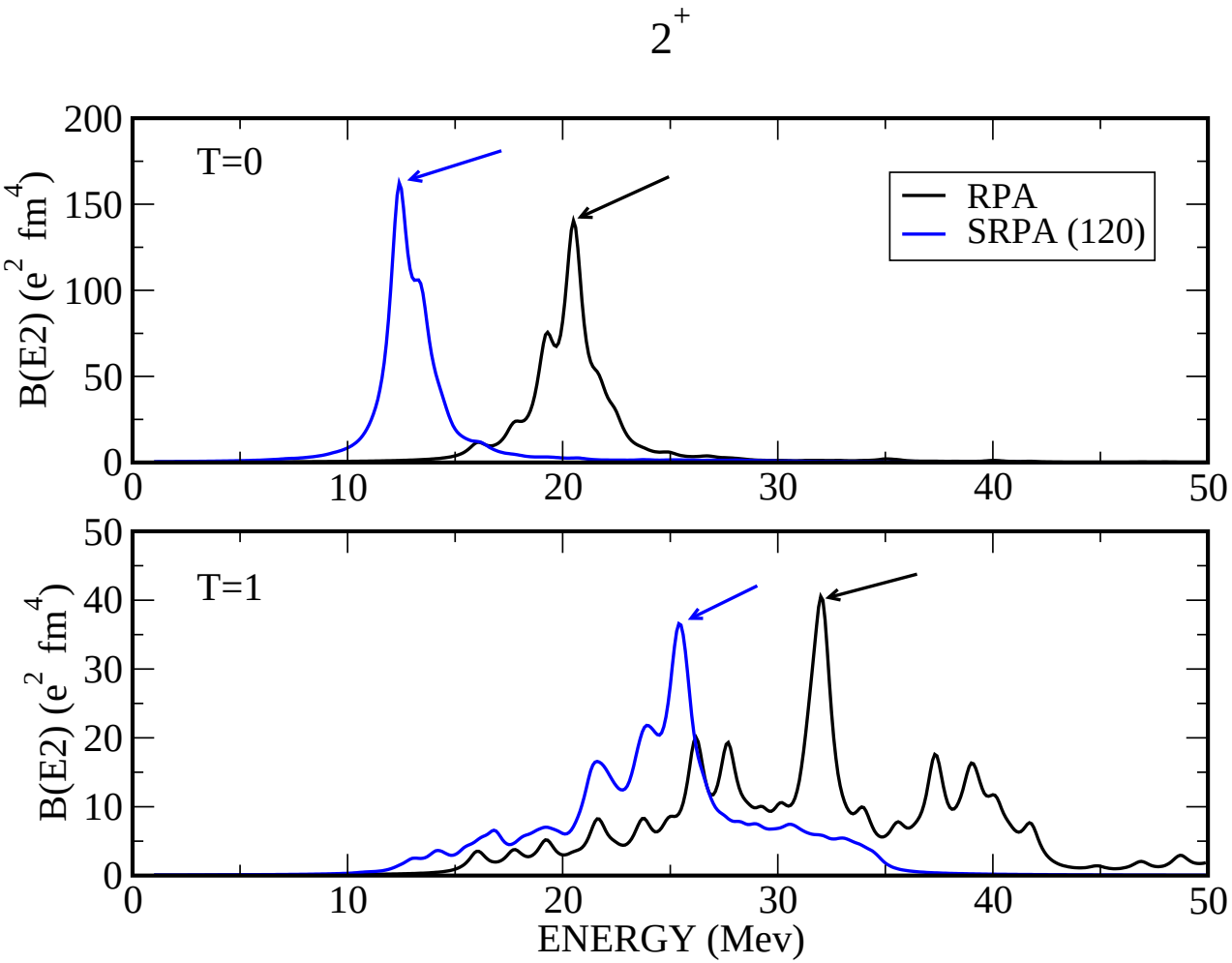
Monopole Case



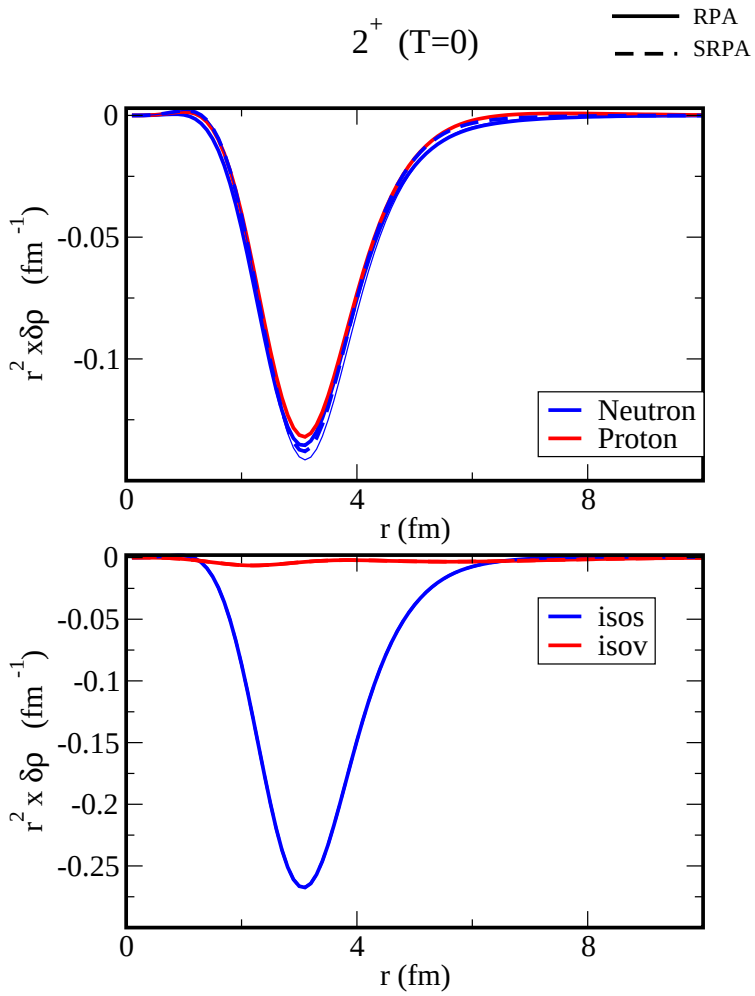
Monopole Transition Densities

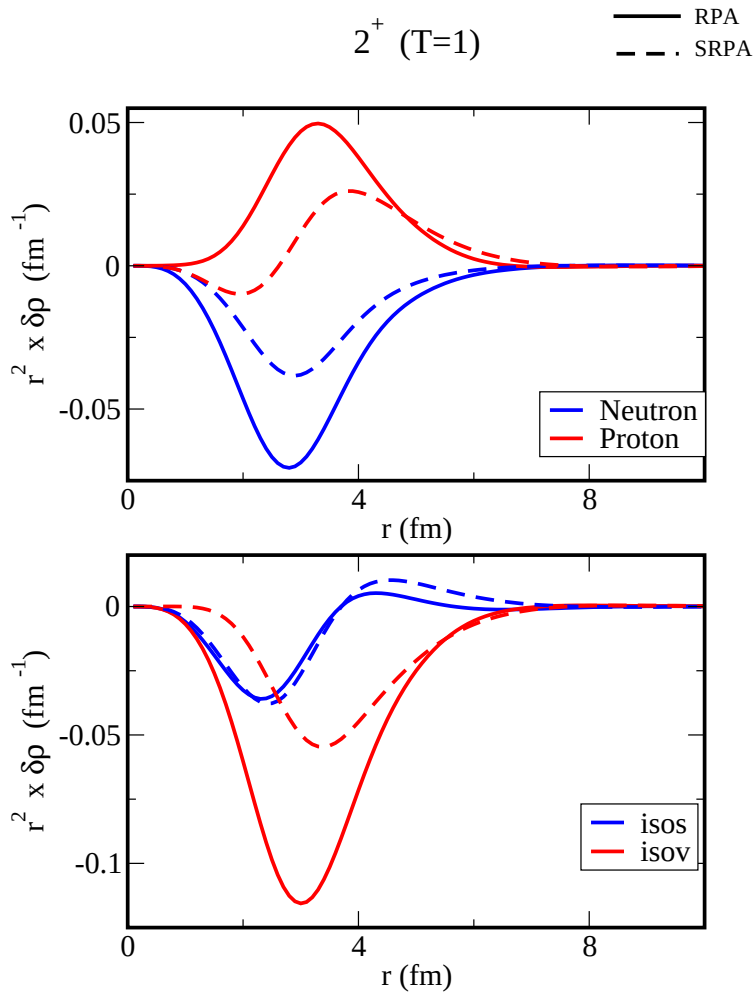


Quadrupole case



Quadrupole Transition Densities





Why Metallic Clusters?

Metallic Clusters

- Metallic Clusters are aggregates of atoms with a well defined size
- The atoms are usually decomposed into **valence electrons** and **ionic cores**

Analogies between metallic clusters and nuclei:

- **Shell Structure and Magic Numbers**
- **Dipole Plasmon**: collective motion of valence electrons against ions

Good Test Laboratory for Many-Body System Studies

- We use Jellium approximation for Ionic structure
- No adjustable parameters
- No use of effective interactions is necessary
- Clearer comparison between different levels of approximation

SRPA in Metallic Clusters

Dipole Plasmon in Na clusters

- A very strong shift of the strength distribution in found in SRPA with respect to the RPA [a]
- The quite good RPA description is completely spoiled
- It has been suggested that QBA is a **more** severe approximation than in RPA [b]

---

[a] D. Gambacurta and F. Catara, Phys. Rev. B 79

[b] K. Takayanagi *et al.*, Nucl. Phys. A477,(1988) 205 G. Lauritsch *et al.*, Nucl. Phys. A509, (1990) 287 A. Mariano *et al.*, Phys. Rev. C49, (1994) 2824, D. Gambacurta *et al.* C73, 024319 (2006)

Extended SRPA: (D. Gambacurta and F. Catara, Phys. Rev. B, (2010))

- No use is made of QBA
- Better description of ground state correlations

Extended SRPA

Extended SRPA

- We introduce the correlated reference state $|\,0\rangle$ (vacuum of the Q's)
- We calculate the double commutators appearing SRPA matrices without any approximation
- The so-obtained terms are contracted with respect to $|\,0\rangle$
- The matrix elements are expressed in terms of the 1-body density matrix ρ
- ρ is assumed to be diagonal $\rho(\alpha,\beta) = \delta_{\alpha\beta} n_\alpha$
- The occupation number n are expressed in term of the X and Y amplitudes by means of the number operator method [a]
- ESRPA: non linear SRPA-like equations

[a] D. J. Rowe, Phys. Rev. **175**, 1283 (1968)

Extended SRPA

SRPA calculations are much more time expensive than the RPA ones

An iterative procedure involving SRPA matrices is not easily affordable

Extended RPA: **ERPA**

- We first apply the procedure discussed in the previous slide just at RPA level
- We obtain non-linear RPA-like equations: **ERPA**
- We solve them via an iterative procedure
- We obtain a set of occupation numbers

Extended SRPA: **ESRPA**

- We use the so obtained occupation numbers in the ESRPA equations

ERPA Equations

ERPA Equations of Motion

$$\begin{pmatrix} A & B \\ -B^* & -A^* \end{pmatrix} \begin{pmatrix} X^{(\nu)} \\ Y^{(\nu)} \end{pmatrix} = \omega_\nu \begin{pmatrix} G & 0 \\ 0 & G^* \end{pmatrix} \begin{pmatrix} X^{(\nu)} \\ Y^{(\nu)} \end{pmatrix}$$

ERPA Matrices

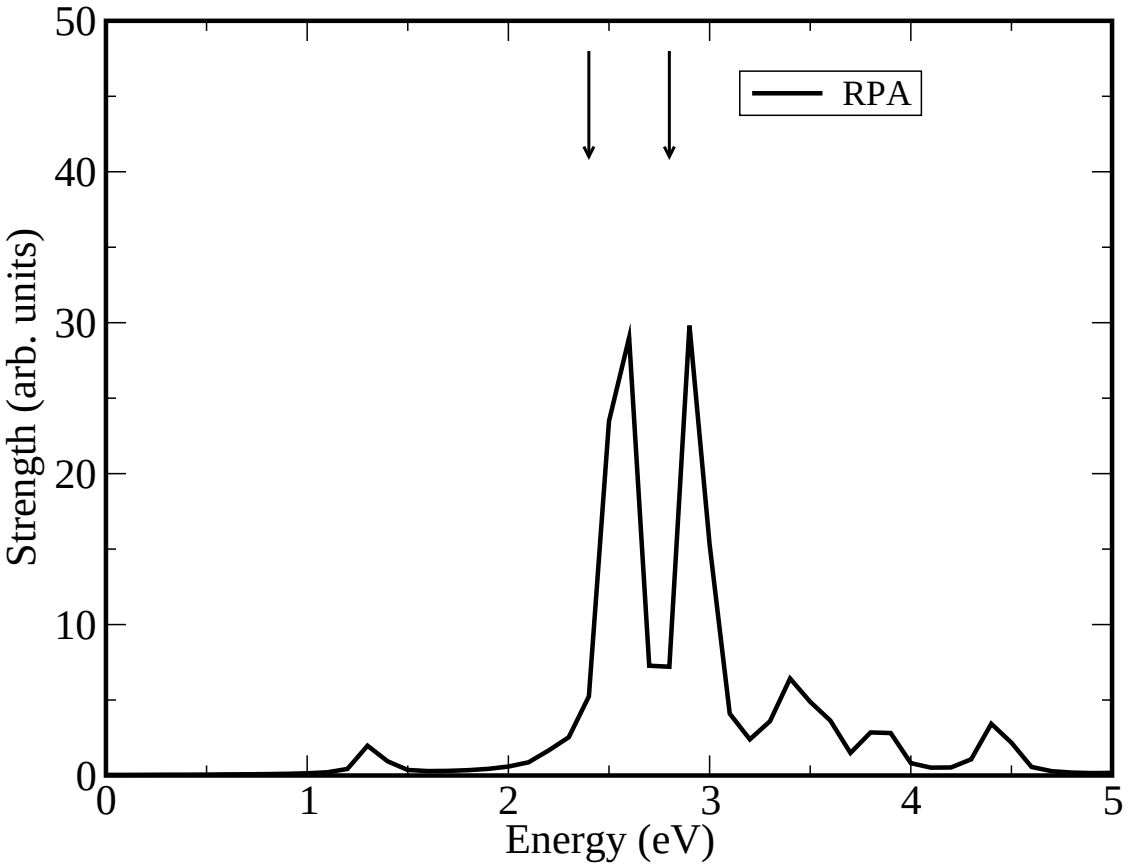
$$A_{ph,p'h'} = \delta_{hh'}\delta_{pp'}(\epsilon_p - \epsilon_h)(n_h - n_p) + \langle ph'|V|hp'\rangle(n_h - n_p)(n_{h'} - n_{p'})$$

$$B_{ph,p'h'} = \langle pp'|V|hh'\rangle(n_h - n_p)(n_{h'} - n_{p'})$$

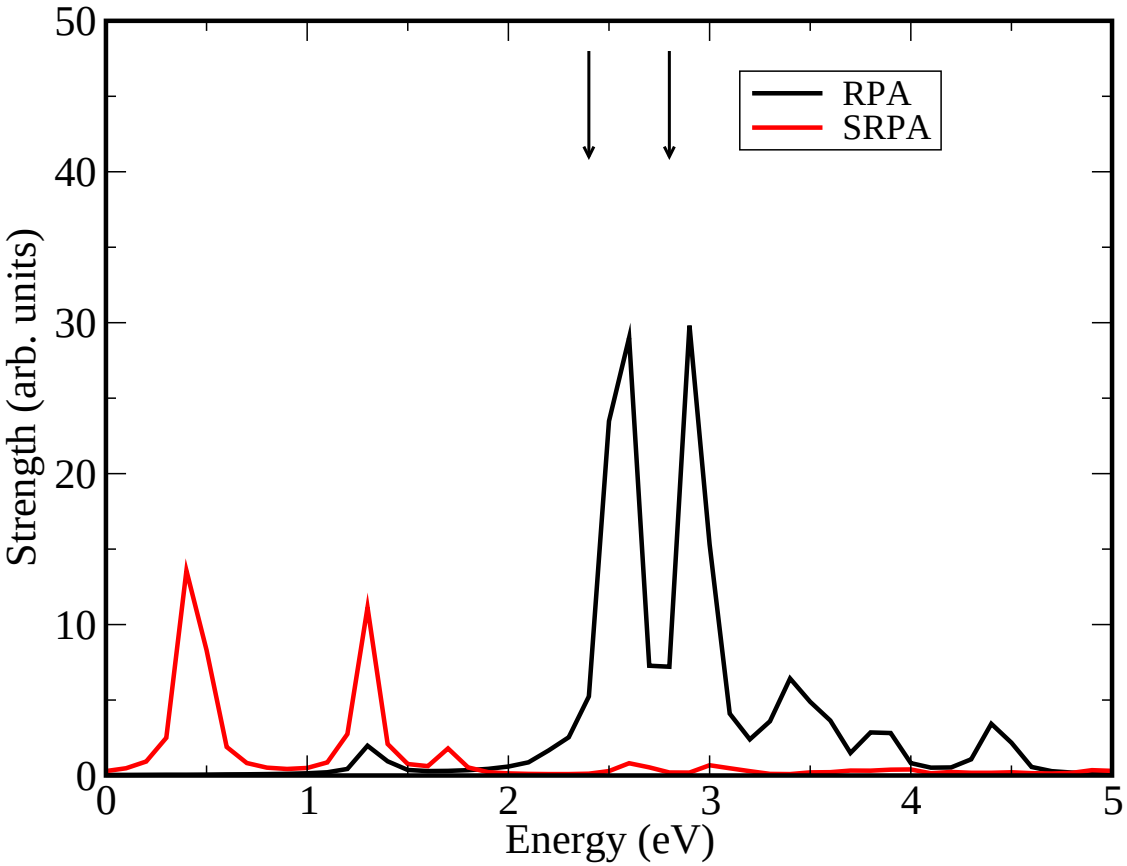
$$G_{ph,p'h'} = \delta_{hh'}\delta_{pp'}(n_h - n_p)$$

$$n_i = n_i(X, Y)$$

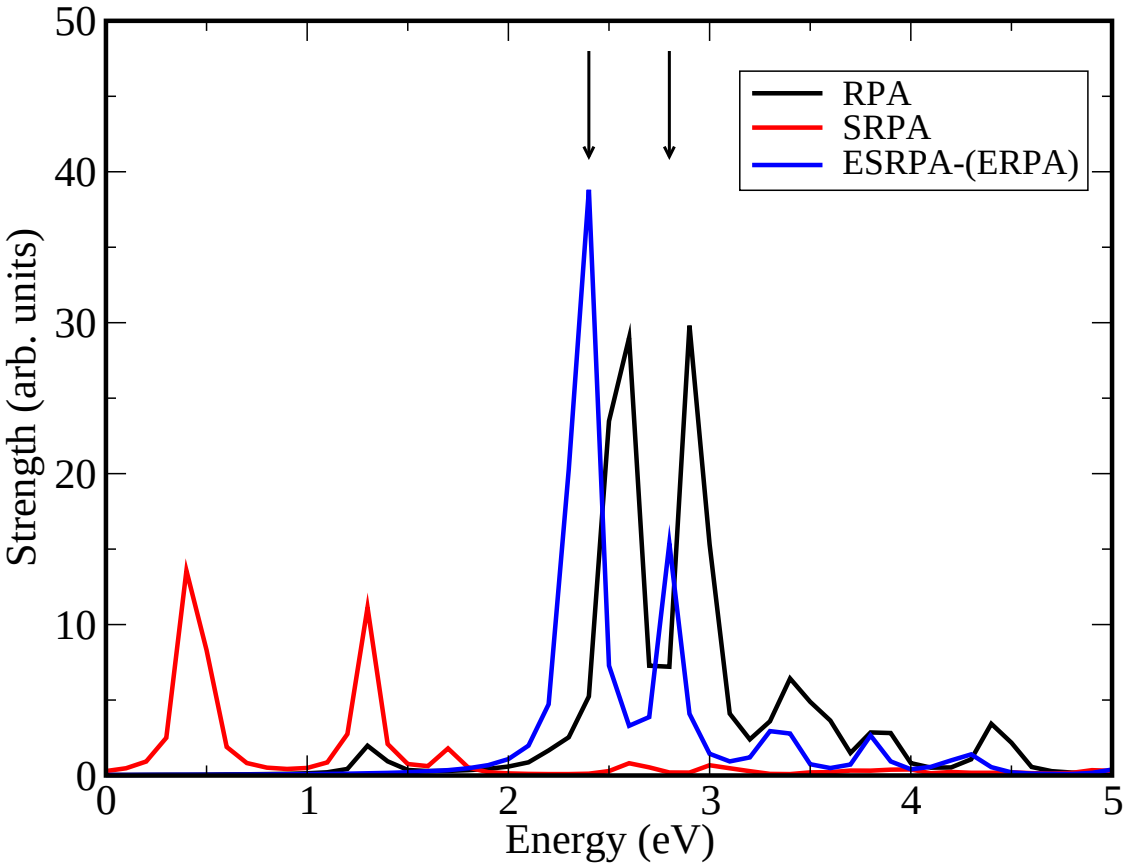
Na_{20} Dipole Strength Distribution



Na_{20} Dipole Strength Distribution



Na_{20} Dipole Strength Distribution



Conclusions and Outlook

Conclusions

- Going from RPA to SRPA we observe mainly two effects:
- (1) Fragmentation of the Strength
- (2) A strong shift of the Strength Distribution towards lower energies
- Rearrangement terms as they came out from RPA seem to be not appropriate in SRPA
- Diagonal Approximation could be not adequate
- Extended SRPA in metallic clusters improves SRPA

Outlook

- Derivation of the Residual Interaction in SRPA with DDF (Work in Progress)
- Study of other nuclei (^{40}Ca)
- SRPA with finite range interaction (Gogny, V-low-k, ..)
- Apply the Extended RPA and SRPA to the nuclear case