Relativistic QRPA with exact coupling to the continuum

Ioannis Daoutidis

IAA, Université Libre Bruxelles

June 9, 2011

Contents of the talk

1. Density Functional Theory in relativistic static phenomena
2. Method to describe nuclear collective phenomena (RPA)
3. Exact treatment of the continuum
4. Results in spherical nuclei and comparison with experiment
5. Conclusions

Density Functional Theory

$$E[\hat{\rho}] = \langle \Psi | H | \Psi \rangle$$ exact!

density matrix $\rho(\mathbf{r}, \mathbf{r}') = \sum_{\mathbf{i=1}}^{\mathbf{A}} |\phi_{\mathbf{i}}(\mathbf{r})\rangle\langle\phi_{\mathbf{i}}(\mathbf{r}')|$

Mean Field

$$\hat{h} = \frac{\delta E}{\delta \hat{\rho}}$$

Eigenfunctions:

$$\hat{h}|\phi_i\rangle = \varepsilon_i|\phi_i\rangle$$

Interaction:

$$V = \frac{\delta^2 E}{\delta \hat{\rho}^2}$$

Density Functional Theory

$$E[\hat{\rho}] = \langle \Psi | H | \Psi \rangle$$ exact!

density matrix $\rho(\mathbf{r}, \mathbf{r}') = \sum_{\mathbf{i}=\mathbf{1}}^{\mathbf{A}} |\phi_{\mathbf{i}}(\mathbf{r})\rangle\langle\phi_{\mathbf{i}}(\mathbf{r}')|$

Mean Field

$$\hat{h} = \frac{\delta E}{\delta \hat{\rho}}$$

Eigenfunctions:

$$\hat{h}|\phi_i\rangle = \varepsilon_i|\phi_i\rangle$$

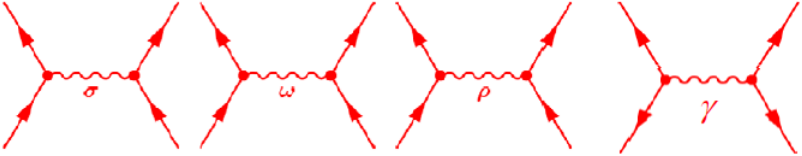
Interaction:

$$V = \frac{\delta^2 E}{\delta \hat{\rho}^2}$$

- Extensions: Pairing correlation (BCS)

Relativistic DFT

Nucleons are coupled by exchange of mesons



$(J^\pi,T)=(0^+,0)$ $(J^\pi,T)=(1^-,0)$ $(J^\pi,T)=(1^-,1)$

$$S(\mathbf{r}) = g_\sigma \sigma(\mathbf{r}) \qquad V(\mathbf{r}) = g_\omega \omega(\mathbf{r}) + g_\rho \vec{\tau}\vec{\rho}(\mathbf{r})\omega(\mathbf{r}) + \mathbf{eA}(\mathbf{r})$$

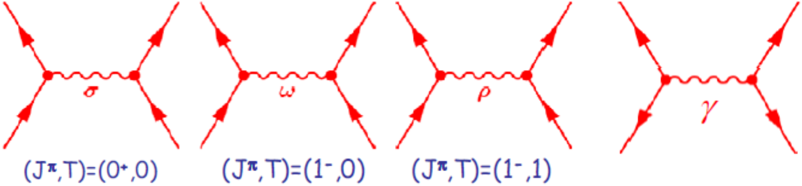
Sigma-meson:
Attractive scalar field

Omega-meson:
short range
repulsive

Rho-meson:
isovector field

Relativistic DFT

Nucleons are coupled by exchange of mesons



$$S(\mathbf{r}) = g_\sigma \sigma(\mathbf{r}) \qquad V(\mathbf{r}) = g_\omega \omega(\mathbf{r}) + g_\rho \vec{\tau}\vec{\rho}(\mathbf{r})\omega(\mathbf{r}) + \mathbf{eA}(\mathbf{r})$$

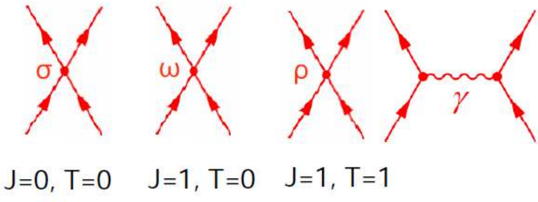
Sigma-meson:
Attractive scalar field

Omega-meson:
short range
repulsive

Rho-meson:
isovector field

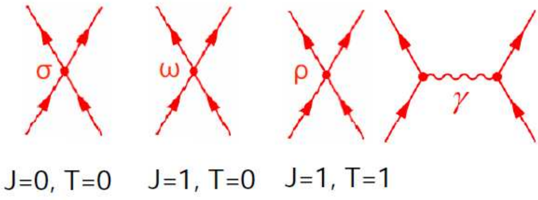
Dirac equation: $[\alpha \cdot p + \beta(m + S(\mathbf{r})) + \mathbf{V}(\mathbf{r})]\, \psi_i(\mathbf{r}) = \varepsilon_\mathbf{i} \psi_\mathbf{i}(\mathbf{r})$

Relativistic Point Coupling



Linear terms $\alpha_S, \alpha_V, \alpha_{TV}$

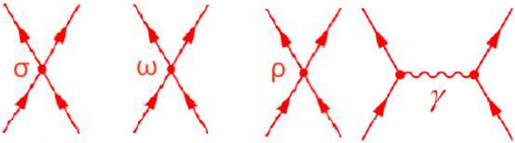
Relativistic Point Coupling



Linear terms $\alpha_S, \alpha_V, \alpha_{TV}$

+ density dependent couplings $\beta_S, \gamma_S, \gamma_V$

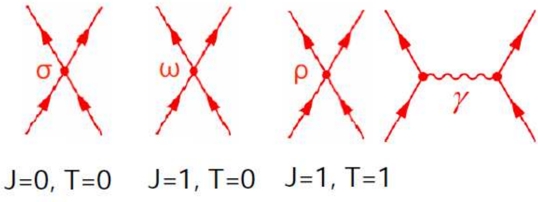
Relativistic Point Coupling



J=0, T=0 J=1, T=0 J=1, T=1

Linear terms $\alpha_S, \alpha_V, \alpha_{TV}$
+ density dependent couplings $\beta_S, \gamma_S, \gamma_V$
+ gradient terms $\delta_S, \delta_V, \delta_{TV}$

Relativistic Point Coupling



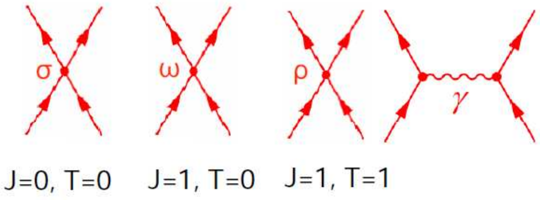
Linear terms $\alpha_S, \alpha_V, \alpha_{TV}$

+ density dependent couplings $\beta_S, \gamma_S, \gamma_V$

+ gradient terms $\delta_S, \delta_V, \delta_{TV}$

$$E[\hat{\rho}]$$

Relativistic Point Coupling



Linear terms $\alpha_S, \alpha_V, \alpha_{TV}$

+ density dependent couplings $\beta_S, \gamma_S, \gamma_V$

+ gradient terms $\delta_S, \delta_V, \delta_{TV}$

$$E[\hat{\rho}]$$

PCF1:Buervenich et al. Phys. Rev. C65, 044308 (2002).
DDPC1:Niksic et al. Phys. Rev. C78,034318 (2008).

Beyond DFT

$\surd$ Ground state properties
(binding energies, nuclear radii, etc.)

X Collective excitations
(surface oscillations, Giant Multipole Resonances)

Beyond DFT

$\surd$ Ground state properties
(binding energies, nuclear radii, etc.)

X Collective excitations
(surface oscillations, Giant Multipole Resonances)

How can we explain reactions that lead to collective excitations from individual motion?

$$\sigma = (2L+1)\pi^2(\hbar\, c)^2 E^{2L-1} S(E)$$

Beyond DFT

$\surd$ Ground state properties
(binding energies, nuclear radii, etc.)

X Collective excitations
(surface oscillations, Giant Multipole Resonances)

How can we explain reactions that lead to collective excitations from individual motion?

$$\sigma = (2L+1)\pi^2(\hbar c)^2 E^{2L-1} S(E)$$

Linear Response Theory

$$S(E) = -\frac{1}{\pi} Im \left[F_{ext} R(E) F_{ext}\right] \qquad F_{ext} = \text{external field}$$

Linear Response Theory

Bethe-Salpeter equation:

$$R(E) = R^0(E) + R^0(E) V_{ph} R(E)$$

Linear Response Theory

Bethe-Salpeter equation:

$$R(E) = R^0(E) + R^0(E)\, V_{ph}\, R(E)$$

Interaction :

$$V_{ph} = \frac{\delta^2 E}{\delta \hat{\rho}^2}$$

Linear Response Theory

Bethe-Salpeter equation:

$$R(E) = R^0(E) + R^0(E)\, V_{ph}\, R(E)$$

Free response function:

$$R^0(E) = ?$$

Interaction :

$$V_{ph} = \frac{\delta^2 E}{\delta \hat{\rho}^2}$$

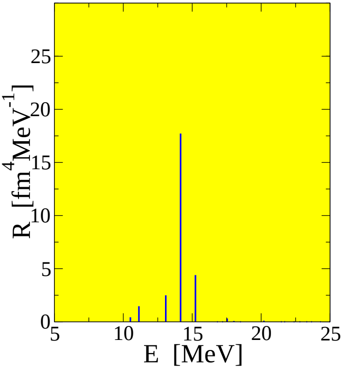
Free response function

$$R^0(E) = \sum_h \langle h|G(E+\varepsilon_h)|h\rangle + b.g.$$

Free response function

$$R^0(E) = \sum_h \langle h | G(E + \varepsilon_h) | h \rangle + b.g.$$

- Spectral representation (Discrete RPA)

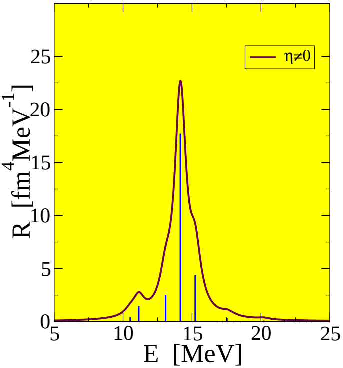


$$G(\mathbf{r}, \mathbf{r}'; \mathbf{E}) = \sum_p^{< E_{max}} \frac{|p\rangle_r \langle p|_{r'}}{E - (\varepsilon_p - \varepsilon_h) + i\eta} + \sum_a^{< E^a_{max}} \frac{|a\rangle_r \langle a|_{r'}}{E - (\varepsilon_a - \varepsilon_h) + i\eta}$$

Free response function

$$R^0(E) = \sum_h \langle h|G(E+\varepsilon_h)|h\rangle + b.g.$$

- Spectral representation (Discrete RPA)



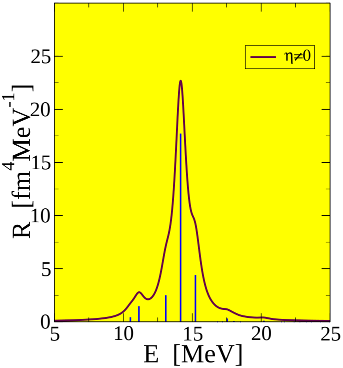
$$G(\mathbf{r},\mathbf{r}';\mathbf{E}) = \sum_p^{<E_{max}} \frac{|p\rangle_r \langle p|_{r'}}{E-(\varepsilon_p-\varepsilon_h)+i\eta} + \sum_a^{<E^a_{max}} \frac{|a\rangle_r \langle a|_{r'}}{E-(\varepsilon_a-\varepsilon_h)+i\eta}$$

- Smearing parameter η is needed to produce a width.

Free response function

$$R^0(E) = \sum_h \langle h|G(E+\varepsilon_h)|h\rangle + b.g.$$

- Spectral representation (Discrete RPA)



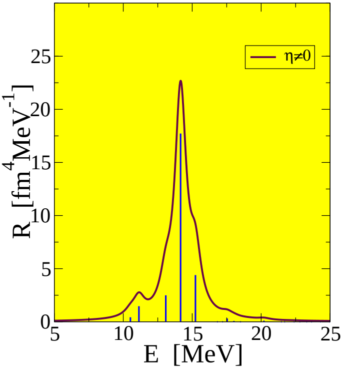
$$G(\mathbf{r},\mathbf{r}';\mathbf{E}) = \sum_p^{<E_{max}} \frac{|p\rangle_r\langle p|_{r'}}{E-(\varepsilon_p-\varepsilon_h)+i\eta} + \sum_a^{<E^a_{max}} \frac{|a\rangle_r\langle a|_{r'}}{E-(\varepsilon_a-\varepsilon_h)+i\eta}$$

- Smearing parameter η is needed to produce a width.
- Truncation of the space involves additional parameters and sets limitations.

Free response function

$$R^0(E) = \sum_h \langle h|G(E+\varepsilon_h)|h\rangle + b.g.$$

- Spectral representation (Discrete RPA)



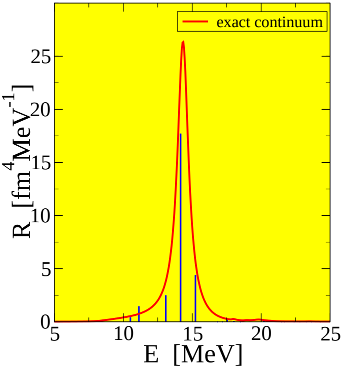
$$G(\mathbf{r},\mathbf{r}';\mathbf{E}) = \sum_p^{<E_{max}} \frac{|p\rangle_r \langle p|_{r'}}{E-(\varepsilon_p-\varepsilon_h)+i\eta} + \sum_a^{<E^a_{max}} \frac{|a\rangle_r \langle a|_{r'}}{E-(\varepsilon_a-\varepsilon_h)+i\eta}$$

- Smearing parameter η is needed to produce a width.
- Truncation of the space involves additional parameters and sets limitations.
- Large amount of terms contributing in R^0 (>2000).

Free response function

$$R^0(E) = \sum_h \langle h | G(E + \varepsilon_h) | h \rangle + b.g.$$

- Non spectral representation (Continuum RPA)

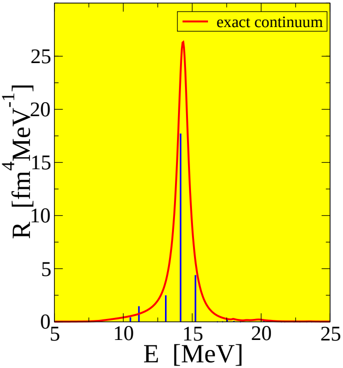


$$G(\mathbf{r}, \mathbf{r}'; \mathbf{E}) = \sum_\kappa \begin{cases} |w_\kappa(\mathbf{r})\rangle\langle \mathbf{u}^*_\kappa(\mathbf{r}')| & r > r' \\ |u_\kappa(\mathbf{r})\rangle\langle \mathbf{w}^*_\kappa(\mathbf{r}')| & r < r' \end{cases}$$

$$|u\rangle = r \begin{pmatrix} j_l(kr) \\ \frac{\kappa}{|\kappa|} \frac{E-V-S}{k} j_{\bar{l}}(kr) \end{pmatrix} \qquad |w\rangle = r \begin{pmatrix} h^{(1)}_l(kr) \\ \frac{\kappa}{|\kappa|} \frac{ikr}{E+2m} h^{(1)}_l(kr) \end{pmatrix}$$

Free response function

$$R^0(E) = \sum_h \langle h|G(E+\varepsilon_h)|h\rangle + b.g.$$



- Non spectral representation (Continuum RPA)

$$G(\mathbf{r},\mathbf{r}';\mathbf{E}) = \sum_\kappa \begin{cases} |w_\kappa(\mathbf{r})\rangle\langle \mathbf{u}^*_\kappa(\mathbf{r}')| & \mathrm{r} > \mathrm{r}' \\ |u_\kappa(\mathbf{r})\rangle\langle \mathbf{w}^*_\kappa(\mathbf{r}')| & \mathrm{r} < \mathrm{r}' \end{cases}$$

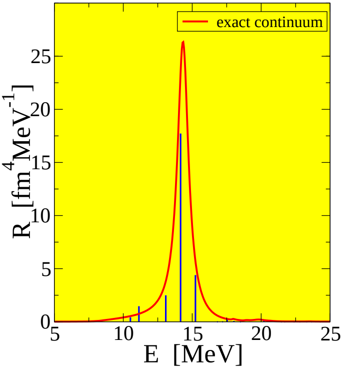
$$|u\rangle = r\begin{pmatrix} j_l(kr) \\ \frac{\kappa}{|\kappa|}\frac{E-V-S}{k} j_{\bar{l}}(kr) \end{pmatrix} \qquad |w\rangle = r\begin{pmatrix} h^{(1)}_l(kr) \\ \frac{\kappa}{|\kappa|}\frac{ikr}{E+2m} h^{(1)}_l(kr) \end{pmatrix}$$

- Small amount of terms contributing in R^0 ($<$50)

Free response function

$$R^0(E) = \sum_h \langle h | G(E + \varepsilon_h) | h \rangle + b.g.$$

- Non spectral representation (Continuum RPA)



$$G(\mathbf{r}, \mathbf{r}'; \mathbf{E}) = \sum_\kappa \begin{cases} |w_\kappa(\mathbf{r})\rangle\langle \mathbf{u}^*_\kappa(\mathbf{r}')| & \mathrm{r} > \mathrm{r}' \\ |u_\kappa(\mathbf{r})\rangle\langle \mathbf{w}^*_\kappa(\mathbf{r}')| & \mathrm{r} < \mathrm{r}' \end{cases}$$

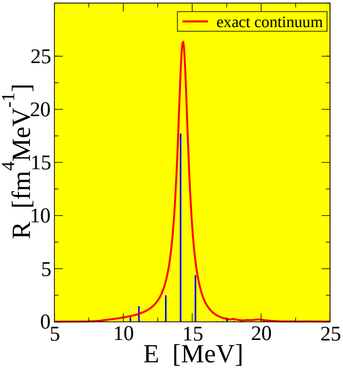
$$|u\rangle = r\begin{pmatrix} j_l(kr) \\ \frac{\kappa}{|\kappa|}\frac{E-V-S}{k} j_{\bar{l}}(kr) \end{pmatrix} \qquad |w\rangle = r\begin{pmatrix} h_l^{(1)}(kr) \\ \frac{\kappa}{|\kappa|}\frac{ikr}{E+2m} h_l^{(1)}(kr) \end{pmatrix}$$

- Small amount of terms contributing in R^0 ($<$50)
- Antiparticle-hole pairs are included effectively.

Free response function

$$R^0(E) = \sum_h \langle h|G(E+\varepsilon_h)|h\rangle + b.g.$$

- Non spectral representation (Continuum RPA)



$$G(\mathbf{r},\mathbf{r}';\mathbf{E}) = \sum_\kappa \begin{cases} |w_\kappa(\mathbf{r})\rangle\langle \mathbf{u}^*_\kappa(\mathbf{r}')| & \text{r} > \text{r}' \\ |u_\kappa(\mathbf{r})\rangle\langle \mathbf{w}^*_\kappa(\mathbf{r}')| & \text{r} < \text{r}' \end{cases}$$

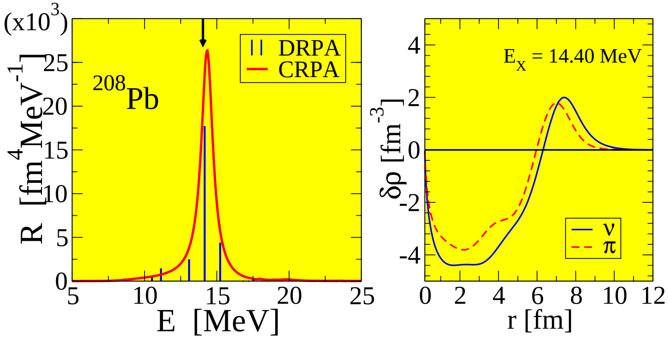
$$|u\rangle = r\begin{pmatrix} j_l(kr) \\ \frac{\kappa}{|\kappa|}\frac{E-V-S}{k} j_{\bar{l}}(kr) \end{pmatrix} \qquad |w\rangle = r\begin{pmatrix} h^{(1)}_l(kr) \\ \frac{\kappa}{|\kappa|}\frac{ikr}{E+2m} h^{(1)}_l(kr) \end{pmatrix}$$

- Small amount of terms contributing in R^0 (<50)
- Antiparticle-hole pairs are included effectively.
- Resonance width is reproduced without smearing parameter (escape width $\Gamma^\uparrow$)

Contents of the talk

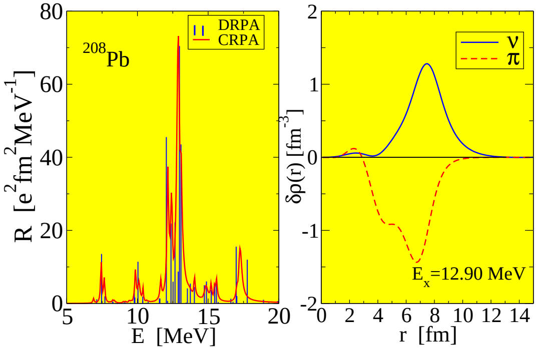
1. Density Functional Theory in relativistic static phenomena,
2. Method to describe nuclear collective phenomena (RPA),
3. Exact treatment of the continuum,
4. Results in spherical nuclei and comparison with experiment,
5. Conclusions.

Isoscalar Monopole Resonance

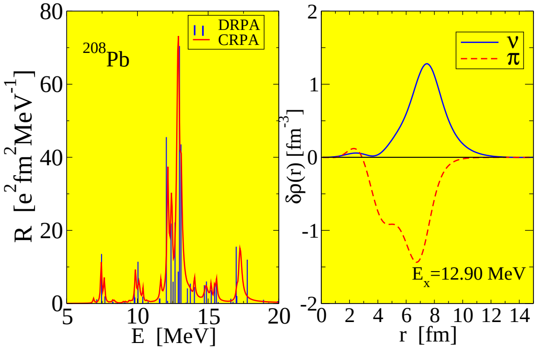


	CRPA	DRPA	Exp.
$\bar{E}$ [MeV]	14.40	14.17	13.96±0.2
Γ [MeV]	0.95		2.88 ±0.2
	CRPA	DRPA	TRK
m_1 $[10^5 MeV fm^4]$	5.448	5.446	5.453

Isovector Dipole Resonance



Isovector Dipole Resonance

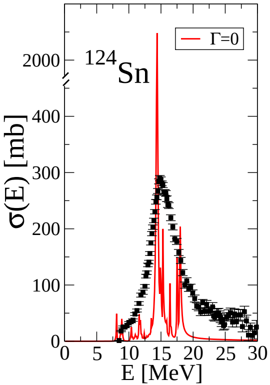


5-10 times faster numerical calculations!

Isovector Dipole Resonance

Coupling to more complex configurations (spreading width):

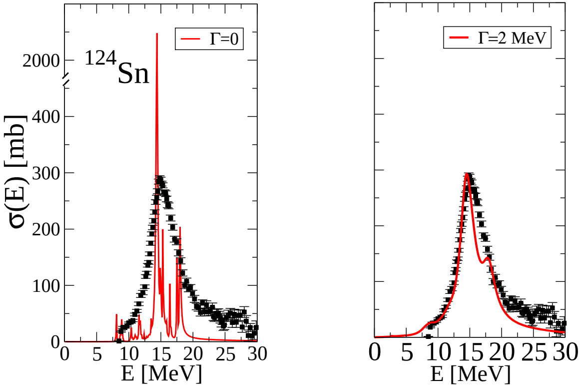
$$G(E) \to G(\omega + i\Gamma), \qquad \Gamma = 0$$



Isovector Dipole Resonance

Coupling to more complex configurations (spreading width):

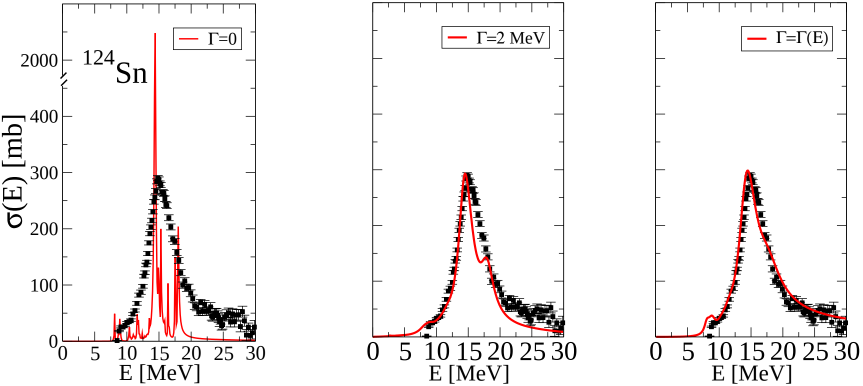
$$G(E) \to G(\omega + i\Gamma), \qquad \Gamma = constant$$



Isovector Dipole Resonance

Coupling to more complex configurations (spreading width):

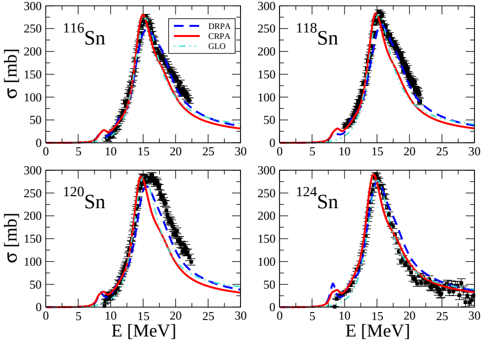
$$G(E) \rightarrow G(\omega + i\Gamma), \qquad \Gamma(E) = \frac{E^2 + 4\pi^2 T^2}{E^2_{GDR}}$$



Isovector Dipole Resonance

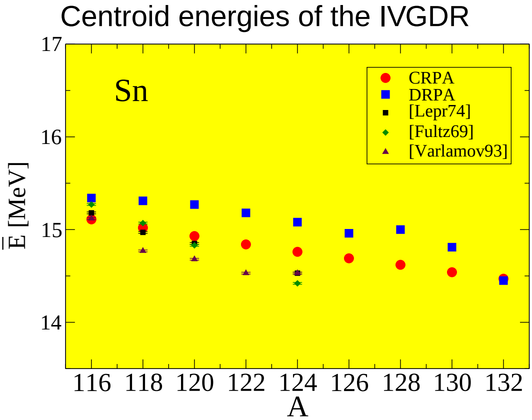
Coupling to more complex configurations (spreading width):

$$G(E) \rightarrow G(\omega + i\Gamma), \qquad \Gamma(E) = \frac{E^2 + 4\pi^2 T^2}{E^2_{GDR}}$$



Exp.: Lepretre et. al. NPA 219,39 (1974)

Isovector Dipole Resonance



Isovector Dipole Resonance

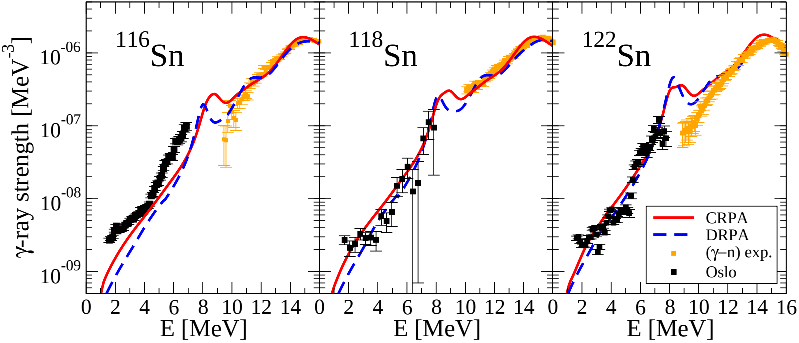
Performance of different point-coupling parameterizations

		DD-PC1	PC-F1	Expt. [MeV]
^{70}Zn	E_0	17.50	16.70	17.25 $\pm$ 0.08
	$\bar{E}$	16.00	15.86	15.68 $\pm$ 0.02
^{94}Zr	E_0	16.60	15.60	16.67 $\pm$ 0.07
	$\bar{E}$	15.90	15.58	16.00 $\pm$ 0.01
^{124}Sn	E_0	15.40	14.40	14.67 $\pm$ 0.08
	$\bar{E}$	14.99	14.70	14.34 $\pm$ 0.02
^{130}Te	E_0	15.30	14.60	14.53 $\pm$ 0.13
	$\bar{E}$	14.96	14.66	14.27 $\pm$ 0.01
^{138}Ba	E_0	15.20	14.40	15.29 $\pm$ 0.15
	$\bar{E}$	14.89	14.55	14.64 $\pm$ 0.01
^{144}Sm	E_0	15.10	14.50	15.37 $\pm$ 0.13
	$\bar{E}$	15.39	14.58	14.77 $\pm$ 0.02
^{208}Pb	E_0	13.60	12.80	13.50 $\pm$ 0.19
	$\bar{E}$	14.40	14.03	13.96 $\pm$ 0.20

Evolution of transition densities

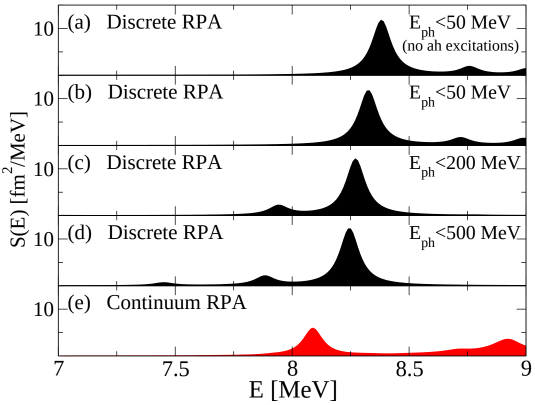
$\rightarrow$ play video. . .

Pygmy Dipole Resonance



I. Daoutidis and S. Goriely, in Prep.
Experiment: Toft et. al. PRC81, 64311 (2010) and PRC83, 44320 (2011)

Pygmy Dipole Resonance



I. Daoutidis and P. Ring PRC 83, 044303 (2011)

Summary

1. Relativistic DFT plus QRPA allows to calculate excitation strength in a fully-self consistent way
2. Continuum QRPA calculations are now possible.
   They appear to be important for :
   - the study of soft modes, sensitive to basis trancation.
   - quantitive improvement of the collective properties
   - determination of the escape width of the resonances
   - considerably reducing the numerical effort

Summary

1. Relativistic DFT plus QRPA allows to calculate excitation strength in a fully-self consistent way
2. Continuum QRPA calculations are now possible. They appear to be important for :
   - the study of soft modes, sensitive to basis trancation.
   - quantitive improvement of the collective properties
   - determination of the escape width of the resonances
   - considerably reducing the numerical effort
3. Gamow-Teller resonances for astrophysical purposes (beta-decay rates, r-process path)
4. Apply Relativistic Hartree Bogoliubov theory to treat pairing correlations at the cases where BCS fails (drip lines, halo nuclei)
5. Extend to include phonon coupling and deformed nuclei

Collaborations:

Peter Ring [Munich]

Stephane Goriely [Brussels]

Daniel Pena Arteaga [Orsay]

George Lalazissis [Thessaloniki]

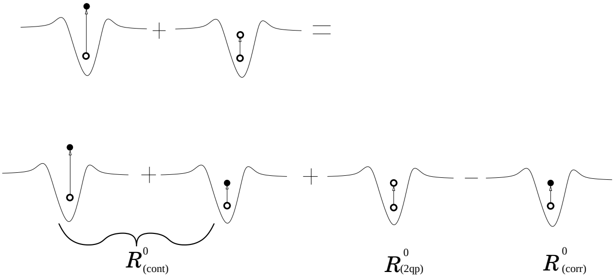
Elena Litvinova [GSI]

Hiroaki Utsunomiya [Kobe]

Thank you

Quasiparticle RPA in the contunuum

Pairing Correlations: BCS



J. Daoutidis and P. Ring PRC 83 (2011)
Non relativistically: K. Hagino and H. Sagawa, Nucl. Phys. A695, 82 (2001).
S. Kamerdzhiev et. al. Phys. Rev. C58, 172 (1998).