RPA for Superfluid Nuclei and Extensions

Paris, Jan. 28, 2010

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Content

- Static density functionals in nuclei
- Time dependent density functionals in nuclei
- Quasiparticle RPA
- Applications:
 - relativistic RPA
 - continuum RPA
 - deformed RPA
 - pn RPA

Extensions

- energy dependent KS-fields
- Mixing of deformed configurations
- Symmetry restoration before variation
- Conclusions and outlook





Density functional theory in nuclei

$$E[\rho] = \langle \Psi | H | \Psi \rangle \approx \langle \Phi | H_{eff}(\rho) | \Phi \rangle$$

 $|\Phi\rangle$ Slater determinant $\iff \rho$ density matrix



 $|\Phi\rangle = \mathcal{A}\{\varphi_1(\mathbf{r}_1)\dots\varphi_i(\mathbf{r}_A)\} \iff \hat{\rho}(\mathbf{r},\mathbf{r}') = \sum_{i=1}^{A} |\varphi_i(\mathbf{r})\rangle\langle\varphi_i(\mathbf{r}')|$

Mean field:Eigenfunctions: $\hat{h} = \frac{\delta E}{\delta \rho}$ $h | \varphi_i \rangle = \varepsilon_i | \varphi_i \rangle$



i=1

Extensions: Pairing correlations, Covariance Relativistic Hartree Bogoliubov (RHB)

Density functionals in nuclei:

- the are based on density dependent two-body interactions H(ρ)
 - on the mean field level they contain also three-body forces
- they are completely phenomenological
 - few parameters are adjusted to binding energies and radii
- they can be represented by zero range forces (and gradient corrections)
 on the mean field level one needs only momenta k < k_F
- for zero range forces **Fock terms** can be absorbed in the parameters
- there are large **spin-orbit** terms
- strong pp-correlations lead in open shell nuclei to superfluidity
 - is treated on the mean field level by Hartree-Fock-Bogoliubov methods

3 types of functionals are presently used:

- non relativistic zero range forces (Skyrme)
- finite range forces of Gaussian shape (Gogny)
- relativistic density functionals (RMF)

Density functionals in superfluid systems:

$$E[\boldsymbol{\rho}, \boldsymbol{\kappa}] = E_{\mathsf{KS}}[\boldsymbol{\rho}] + E_{\mathsf{pair}}[\boldsymbol{\kappa}]$$

where

$$\boldsymbol{\rho} = \langle a^{\dagger}a \rangle \qquad \boldsymbol{\kappa} = \langle a^{\dagger}a^{\dagger} \rangle$$

$$\mathcal{R}=\left(egin{array}{cc} oldsymbol{
ho} & \kappa \ -\kappa^* & -oldsymbol{
ho}^* \end{array}
ight)$$

and the Kohn-Sham equations are of the form

Valatin density

$$\begin{pmatrix} \mathbf{h}_{\mathsf{KS}} - \mu & \mathbf{\Delta} \\ -\mathbf{\Delta}^* & -\mathbf{h}_{\mathsf{KS}}^* + \mu \end{pmatrix} \begin{pmatrix} U_k(\mathbf{r}) \\ V_k(\mathbf{r}) \end{pmatrix} = E_k \begin{pmatrix} U_k(\mathbf{r}) \\ V_k(\mathbf{r}) \end{pmatrix}$$

with

$$h_{\rm KS} = \frac{\delta E}{\delta \rho}, \qquad \Delta = \frac{\delta E}{\delta \kappa}$$

Relativistic Kohn-Sham equations:

$$\begin{pmatrix} m - \mathbf{S} + \mathbf{V} & \vec{\sigma}\vec{p} \\ \vec{\sigma}\vec{p} & -m + \mathbf{S} + \mathbf{V} \end{pmatrix} \begin{pmatrix} f_i \\ g_i \end{pmatrix} = \varepsilon_i \begin{pmatrix} f_i \\ g_i \end{pmatrix}$$

scalar potential:
$$S(\mathbf{r}) = G_{\sigma}\rho_s(\mathbf{r}) = G_{\sigma}\sum_{i=1}^{A} (|f_i(\mathbf{r})|^2 - |g_i(\mathbf{r})|^2 \approx 400 \text{ MeV}$$
vector potential: $V(\mathbf{r}) = G_{\omega}\rho(\mathbf{r}) = G_{\omega}\sum_{i=1}^{A} (|f_i(\mathbf{r})|^2 + |g_i(\mathbf{r})|^2 \approx 350 \text{ MeV}$ density dependent couplings: $\mathbf{G} = \mathbf{G}(\mathbf{p})$ rearrangement terms!

Relativistic potentials





Walecka model



- the basis is an effective Lagrangian with all relativistic symmetries
- it is used in a mean field concept (Hartree-level)
- with the no-sea approximation



Effective density dependence:

The basic idea comes from ab initio calculations density dependent coupling constants include Brueckner correlations and threebody forces



Manakos and Mannel, Z.Phys. 330 , 223 (1988)		
Bürvenich, Madland, Maruhn, Reinhard, PRC 65, 044308 (2002):	PC-F1	
Niksic, Vretenar, P.R., PRC 78, 034318 (2008):	DD-PC1	

rms-deviations:masses: $\Delta m = 900 \text{ keV}$ radii: $\Delta r = 0.015 \text{ fm}$

Lalazissis, Niksic, Vretenar, Ring, PRC 71, 024312 (2005)



Comparison with ab initio calculations:



we find excellent agreement with ab initio calculations of Baldo et al.

Fit to ab-initio results

point coupling model is fitted to microscopic nuclear matter:



Static density functionals in nuclei

Time dependent density functionals in nuclei

Quasiparticle RPA

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Time dependent mean field theory:

$$\int dt \left\{ \langle \Phi(t) | i \partial_t | \Phi(t) \rangle - E[\hat{\rho}(t)] \right\} = 0$$
$$i \partial_t \hat{\rho} = \left[\hat{h}(\hat{\rho}) + \hat{f}, \hat{\rho} \right]$$

$$i\partial_t \psi(t) = \left[\left(\vec{\alpha} (\vec{p} - \vec{V}(t)) + V(t) + \beta (m - S(t)) \right] \psi(t) \right]$$

We neglect retardation and find for the fields at each time-step:

$$S(t) = G_{\sigma}\rho_s(t)$$
$$V(t) = G_{\omega}\rho(t)$$
$$\vec{V}(t) = G_{\omega}\vec{j}(t)$$

and similar equations for the isovector and electromagnetic-fields



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Small amplitude limit gives RPA:Small amplitude limit:
$$\delta \rho_{ph}, \delta \rho_{ah}$$
 $\hat{\rho}(t) = \hat{\rho}^{(0)} + \delta \hat{\rho}(t)$ $\begin{pmatrix} A & B \\ -B^* & -A^* \end{pmatrix} \begin{pmatrix} X \\ Y \end{pmatrix} = \hbar \omega \begin{pmatrix} X \\ Y \end{pmatrix}$ ground-state density $\delta \rho_{hp}, \delta \rho_{hc}$ **RPA matrices:** $\delta \rho_{hp}, \delta \rho_{hc}$ $A_{minj} = (\epsilon_n - \epsilon_i) \delta_{mn} \delta_{ij} + \frac{\partial h_{mi}}{\partial \rho_{nj}}, \quad B_{minj} = \frac{\partial h_{mi}}{\partial \rho_{jn}}$ \longrightarrow the same effective interaction determines
the Dirac-Hartree single-particle spectrum
and the residual interactionIn superfluid systems: quasiparticle RPA



Relativistic (Q)RPA calculations of giant resonances



Linear response theory:

Strength function:

Response function:

$$S(\omega) = -\frac{1}{\pi} \operatorname{Im} R_{FF}(\omega),$$

without interaction: $|\mu|$

$$R_{cc'}(\omega) = \sum_{\mu>0} \frac{\langle 0|Q_c^{\dagger}|\mu\rangle\langle\mu|Q_{c'}|0\rangle}{\omega - \Omega_{\mu} + i\eta} - \frac{\langle\mu|Q_c^{\dagger}|0\rangle\langle0|Q_{c'}|\mu\rangle}{\omega + \Omega_{\mu} + i\eta}$$
$$|\mu\rangle \quad \rightarrow \quad |ph\rangle, \qquad \Omega_{\mu} \quad \rightarrow \quad \epsilon_p - \epsilon_h$$
$$R_{cc'}^0(\omega) = \sum_{i} \frac{\langle h|Q_c^{\dagger}|p\rangle\langle p|Q_{c'}|h\rangle}{\omega - \epsilon_p + \epsilon_h} - \dots$$

separable interaction:

$$V^{ph}(1,2) = \sum_{c} \int_{0}^{\infty} dr \ Q_{c}^{(1)}(r) \ \upsilon_{c}(r) \ Q_{c}^{\dagger(2)}(r)$$

lin. Bethe Salpeter Eq:
$$R(\omega) = R^0(\omega) + R^0(\omega)V^{ph}R(\omega)$$

 $R(\omega) = \frac{1}{1 - R^0 V} R^0 = \frac{1}{R^{0-1} - V}$ solution by inversion: $\overline{\omega - \begin{pmatrix} A & B \\ -B^* & -A^* \end{pmatrix}}$ in the ph-basis: Treatment of the continuum: $R^{0}_{cc'}(\omega) = \sum_{ph} \frac{\langle h | Q^{\dagger}_{c} | p \rangle \langle p | Q_{c'} | h \rangle}{\omega - \epsilon_{p} + \epsilon_{h}} - \dots$ Bertsch 1974 $= \sum_{\mathbf{r}} \langle h | \mathbf{Q}_{c}^{\dagger} \frac{1}{\omega + \epsilon_{h} - \hat{h}_{D}} \mathbf{Q}_{c'} | h \rangle - \dots$ $= \sum_{h} \langle h | Q_c^{\dagger} G(\omega + \epsilon_h) Q_{c'} | h \rangle - \dots$ single particle Greens function:

$$G(E) = \frac{1}{E - \hat{h}_D} \qquad \left(E - \hat{h}_\kappa(r)\right) G_\kappa(r, r'; E) = \delta(r - r')$$

,



peak energy:

escape width:







Vibrations in deformed nuclei



isovector-dipole response in ¹⁰⁰Mo









response of the nucleus to an incoming particle







Spin-Isospin Resonances: IAR - GTR



Isobaric Analog Resonance: IAR

PR C69, 054303 (2004)





PR C69, 054303 (2004)



Distribution of cross section over multipolarities



Cross section (v_e,e⁻) averaged over supernova neutrino flux



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Problems with mean field:

- no fluctuation in transitional nuclei
- no energy dependence of the self energy
- symmetry violations have to be restored
- no spectroscopy
- • • • •

Particle-vibrational coupling: energy dependent self-energy



Density functional theory - Landau-Migdal theory

Distribution of single-particle strength in ²⁰⁹Bi



RPA workshop, UPMC Paris 6, Jan. 25-29, 2009

Single particle spectrum in the Pb region



Two-body problem: from self-energy to effective interaction



E. Litvinova:



Parameters of Lorentz distribution* (GDR)

		<E $>$ (MeV)	Γ (MeV)	EWSR (%)	
	RRPA	12.9	2.0	128	
208Pb	RRPA-PC	13.7	4.3	134	
	Exp. $[1]$	13.4	4.1		
	RRPA	14.5	2.6	126	
¹³² Sn	RRPA-PC	15.1	4.4	131	
	Exp. $[2]$	16.1(7)	4.7(2.1)		
48.11:	RRPA	17.9	3.1	119	
	RRPA-PC	18.6	5.1	125	
465	RRPA	17.9	3.2	122	
Te	RRPA-PC	18.7	5.5	128	
*Avoraging interval: 0.30 MoV [1] Reference Input Parameter Library, Versio				Parameter Library, Version	
			[2] Adrich et al., PRL 95 , 132501 (2005).		



Generator Coordinate Method (GCM)

Constraint Hartree Fock produces wave functions depending on a generator coordinate q



1.6

2.4

0.8

q (b)

²⁴Mg

GCM wave function is a superposition of Slater determinants

Hill-Wheeler equation:

$$\int dq' \left[\left\langle q | H | q' \right\rangle - E \left\langle q | q' \right\rangle \right] f(q') = 0$$

0

20

16

12

-1.6

-0.8

E (MeV)

$$\left|\Psi\right\rangle = \int dq f(q) \hat{P}^{N} \hat{P}^{I} \left|q\right\rangle$$

Quantum phase transitions and critical symmetries



RPA workshop, UPMC Paris 6, Jan. 25-29, 2009



GCM: only one scale parameter: X(5): two scale parameters:

E(2₁) E(2₁), BE2(2₂ \rightarrow 0₁)

Problem of GCM at this level:

restricted to y=0

AGP and number projected HFB:

AGP is equivalent to number projected HFB (variation after projection: VAP)

$$|AGP\rangle = (C^{\dagger})^{\frac{N}{2}}|0\rangle = \hat{P}^{N}e^{C^{\dagger}}|0\rangle = \hat{P}^{N}|\Phi\rangle$$

with

$$C^{\dagger} = \sum_{ik} C_{ik} a_i^{\dagger} a_k^{\dagger}$$

The coefficients C_{ik} are variational parameters and Φ is a generalized Slater determinant.

The AGP-energy it the number projected HFB-energy.

$$E_{AGP}[\mathcal{R}] = E^{N}[\mathcal{R}] = \frac{\langle \Phi | H\hat{P}^{N} | \Phi \rangle}{\langle \Phi | \hat{P}^{N} | \Phi \rangle}$$

where \mathcal{R} is the Valatin density. This is an intrinsic density. The corresponding projected HFB-Field is

$$\mathcal{H} = \frac{\delta E^N[\mathcal{R}]}{\delta \mathcal{R}}$$

i.e. we need the analytic dependence of $E^N[\mathcal{R}]$ on \mathcal{R}

projected density functionals:

$$E^{I}[\rho] = \langle \Phi | H \hat{P}^{I} | \Phi \rangle$$

where H is an effective Hamiltonian.

The projected HF (or KS) field is given by

$$h_{KS}^{I} = \frac{\delta E^{I}}{\delta \rho}$$

The generalized Wick theorem shows, that $E^{I}[\rho]$ is an integral over the rotational angle α and it depends on the mixed density

$$\rho(\boldsymbol{\alpha}) = \langle \boldsymbol{\Phi} | a^{\dagger} a e^{i \boldsymbol{\alpha} \hat{J}} | \boldsymbol{\Phi} \rangle.$$

It can be shown that the mixed density can be expressed analytically by the intrinsic density

$$\rho(\alpha) = e^{i\alpha J} \rho (1 + (e^{i\alpha J} - 1)\rho)^{-1}$$

Sheikh, P.R., PRC 78, 14312 (2008)







vinding energies

rms-radii

L. Lopes, PhD Thesis, TUM, 2002

Conclusions:

Phenomenological DFT in nuclei produces exellent results

- static: binding energies, radii, deformations,
- quasistatic: treatment of rotational excitations in the rotating frame
- dynamic: QRPA reproduces positions collective excitations and the response of the nuclear systems to external fields

Beyond mean field:

- energy dependence of the self energy reduces the shell gap
- and allows to calculate the width of giant resonances
- configuration mixing of def. states describes fluctuations and phase transitions
- restoration of symmetries allows to calculate spectroscopic properties

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