



Center for
Molecular Modeling

Faddeev Random Phase Approximation (FRPA): From Nuclei to Molecules

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ECT* Workshop: Reactions and Nucleon Properties in Rare
Isotopes
April 8, 2010

Outline

1 Motivation

2 Theory

- Dyson Equation
- Random Phase Approximation
- Faddeev Equations
- Workflow

3 Results

- Dissociation of H_2
- Ground state energies and ionization energies

4 Conclusions & Outlook



What is FRPA?

It is a Green's function method that uses
Faddeev equations to couple
Random Phase Approximation (RPA) interactions
in a consistent way and to sum them to an infinite order



Motivation

Gives good results in finite systems

- Algebraic Diagrammatic Construction Method to 3rd order (ADC(3)) is fully included
- same physics as GW is included
- good for nuclei and atoms

Supposed to give good results in infinite systems

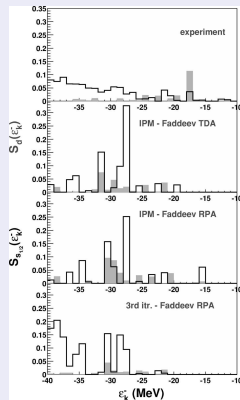
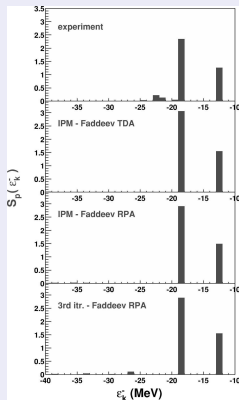
- RPA finds correct plasmon pole for the electron gas



Results from nuclear physics

^{16}O

Phys. Rev. C 65, 064313 (2002)



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Results from atomic physics

Ne in a HF+continuum basis set

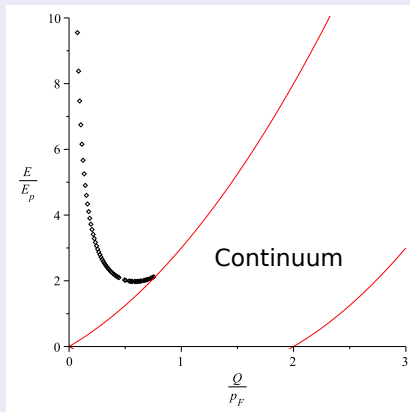
Phys. Rev. A 76, 052503 (2007)

	FTDA	FTDAc	FRPA	FRPAc	exp
2p	-0.870	-0.808	-0.799	-0.801	-0.793
2s	-1.802	-1.804	-1.792	-1.795	-1.782
1s	-32.136	-32.142	-32.097	-32.104	-31.70
E_0	-128.863	-128.883	-128.857	-128.888	-128.928



TDA fails in extended systems

Plasmon Pole



$$\lim_{Q \rightarrow 0} \text{Re}(\Pi_{TDA}(\mathbf{Q}, E)) \sim A \frac{Q}{E} + B \frac{Q^2}{E^2}$$

$$\lim_{Q \rightarrow 0} \text{Re}(\Pi_{RPA}(\mathbf{Q}, E)) \sim C \frac{Q^2}{E^2}$$

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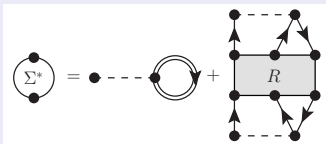
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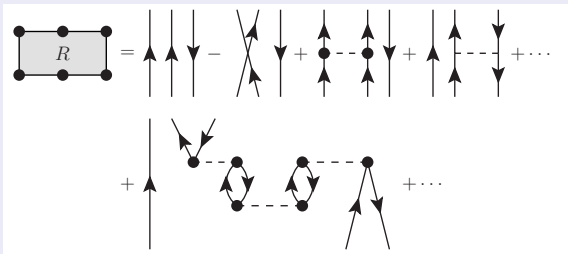


Expansion of self-energy in 2p1h and 2h1p space

FRPA



Diagrams



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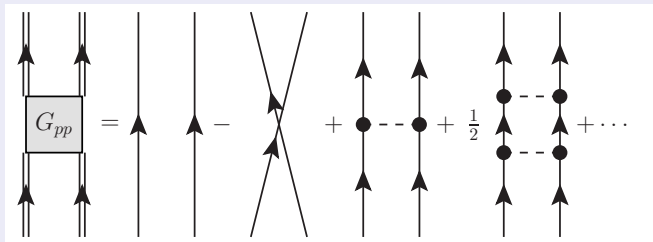
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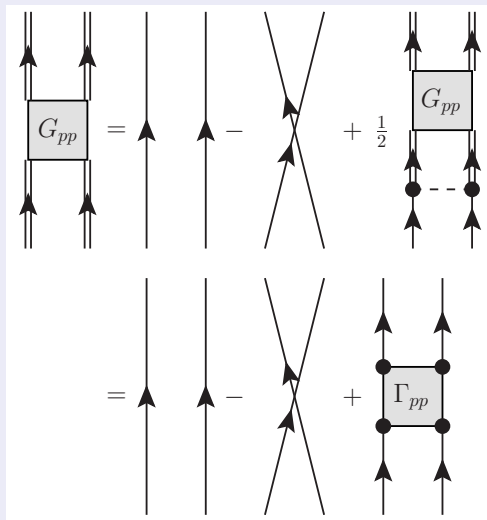
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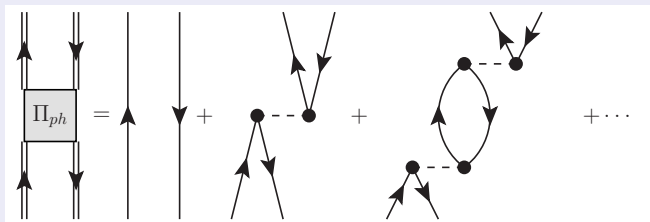
Diagrams



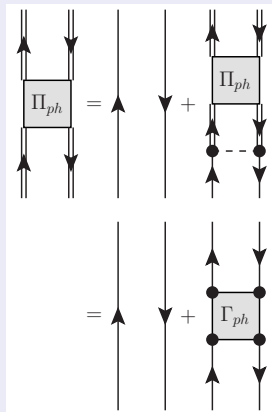
Self-consistent Diagrams



Diagrams



Self-consistent Diagrams



Properties of RPA

- Infinite summation
- Positive and negative energies \Leftrightarrow TDA
- Screened interactions
- Supposed cancellation of omitted diagrams



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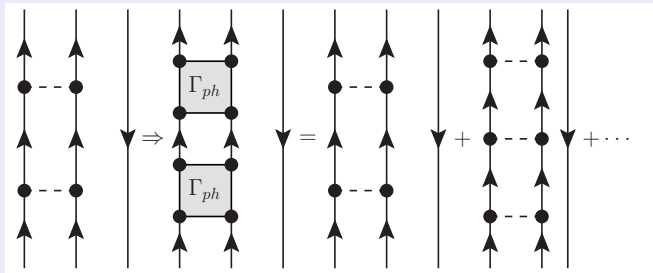
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Substituting RPA into R?

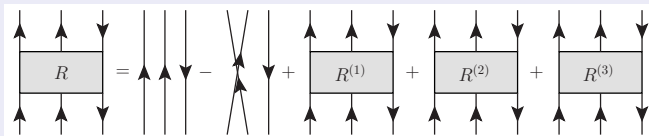
Problem



Already included in RPA diagrams!

Faddeev Technique

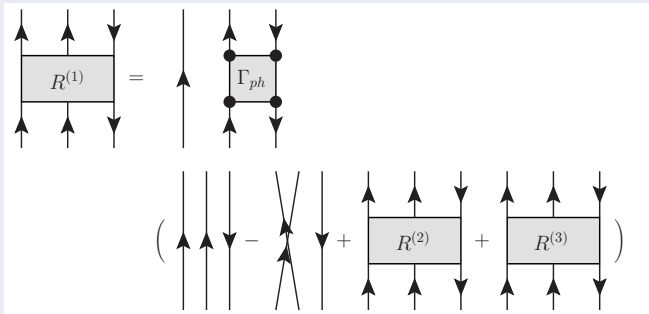
Splitting R



- Derived from 3-body Scattering

Faddeev Technique

Meaning $R^{(i)}$

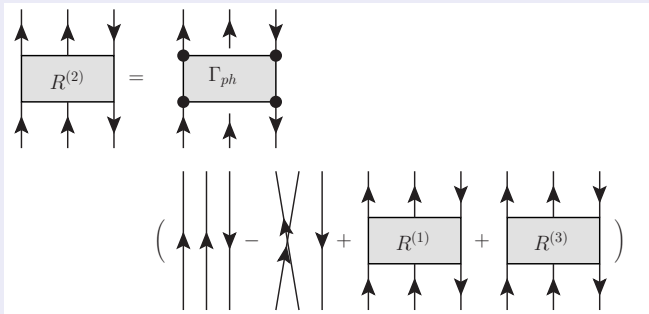


Properties

- pp- and ph-RPA on same footing
- respecting Pauli-principle

Faddeev Technique

Meaning $R^{(i)}$

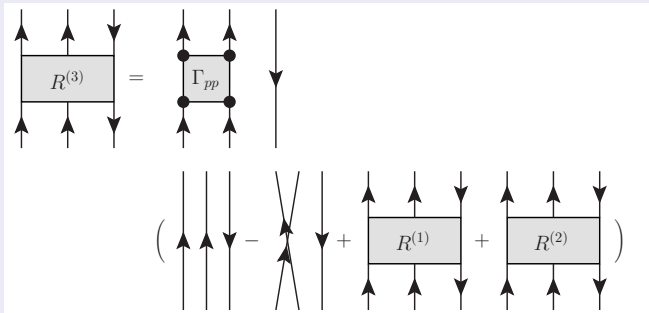


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Faddeev Technique

Meaning $R^{(i)}$



Properties

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Workflow

Diagonalization non-hermitian matrix

- 2p1h and 2h1p poles & amplitudes
- possibly complex



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Removal of spurious solutions

⇒ Reduces basis to normal size



Workflow

Diagonalization non-hermitian matrix

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Removal of spurious solutions

⇒ Reduces basis to normal size

Coupling to single-particle space

$$\begin{pmatrix} \Sigma_{HF} & U_{p/h,2p1h} & U_{p/h,2h1p} \\ U_{2p1h,p/h} & \omega_{2p1h} & 0 \\ U_{2h1p,p/h} & 0 & \omega_{2h1p} \end{pmatrix} \begin{pmatrix} x_{p/h} \\ x_{2p1h} \\ x_{2h1p} \end{pmatrix} = \omega \begin{pmatrix} x_{p/h} \\ x_{2p1h} \\ x_{2h1p} \end{pmatrix}$$

- No (new) complex eigenvalues possible
- Iterative procedure Σ_{HF}

Diatomic molecules

Exploiting symmetry

- Cylindrical symmetry \Rightarrow fixed rotational quantum number
- pp- and ph-RPA phonons with fixed M
- 2p1h and 2h1p states with fixed M
- Restricted to M of single-particle base
- Speedup of Factor 50-100



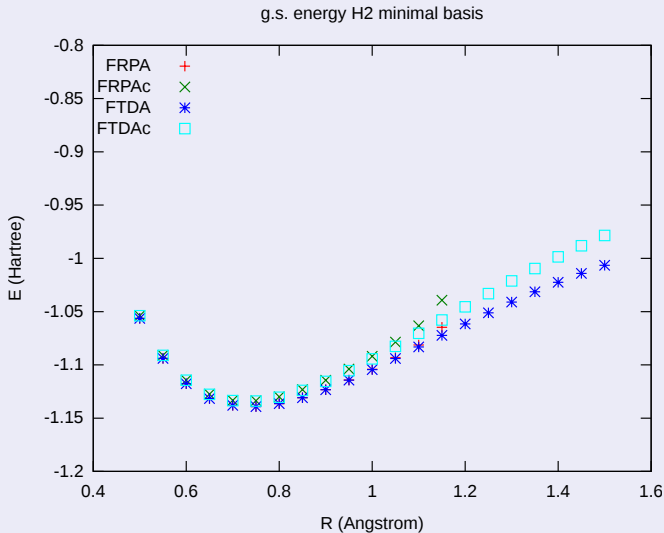
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Dissociation of H₂

H₂ in a minimal basis set



Hartree-Fock instability

- HF ground state = 1 Slater
- Dissociation into two uncharged H = 2 Slaters
- ph-Excitation becomes lower in energy



Hartree-Fock instability

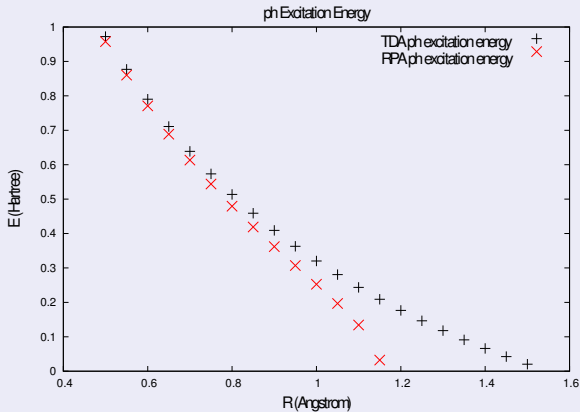
- HF ground state = 1 Slater
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⇒ Breakdown of RPA



Breakdown of RPA

Instability of HF-g.s. to ph excitation



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Results for diatomic molecules

HX

		FTDA	FTDAc	FRPA	FRPAc	CCSD(T)	exp
H ₂ :	E_0	-1.170	-1.161	-1.170	-1.161	-1.164	-
	r_0	0.770	0.757	0.769	0.757	0.761	0.741
	I	0.594	0.589	0.594	0.589	0.583	-
HF:	E_0	-100.173	-100.228	-100.175	-100.224	-100.228	-
	r_0	0.897	0.913	0.904	0.916	0.920	0.917
	I	0.572	0.571	0.577	0.577	0.628	0.592
HCl:	E_0	-460.295	-460.293	-460.258	-460.256	-460.254	-
	r_0	1.314	1.297	1.314	1.293	1.290	1.275
	I	0.457	0.450	0.457	0.450	0.471	-

E_0 = g.s. energy, r_0 = equilibrium distance, I = ionization energy



Results for diatomic molecules

N=14

		FTDA	FTDAc	FRPA	FRPAc	CCSD(T)	exp
BF:	E_0	-124.331	-124.365	-124.332	-124.368	-124.380	-
	r_0	1.285	1.284	1.305	1.285	1.295	1.267
	I	0.417	0.395	0.431	0.402	0.406	-
CO:	E_0	-113.096	-113.037	-113.100	-113.048	-113.055	-
	r_0	1.140	1.130	1.133	1.123	1.145	1.128
	I	0.529	0.503	0.523	0.494	0.550*	0.515
N ₂ :	E_0	-	-109.258	-	-109.272	-109.276	-
	r_0	-	1.104	-	1.106	1.119	1.098
	I	-	0.565	-	0.544	0.602*	0.573

E_0 = g.s. energy, r_0 = equilibrium distance, I = ionization energy



Evaluation

- Competitive accuracy, certainly for bigger systems
- Complex eigenvalues are a big problem

Future

- Fragmentation might solve complex eigenvalues
- ERPA can form an extension
- Infinite systems are still a big challenge



Reading

- theory** C. Barbieri, W.H. Dickhoff, Phys. Rev. C 63, 034313 (2001)
- nuclei** C. Barbieri, W.H. Dickhoff, Phys. Rev. C 65, 064313 (2002)
- atoms** C. Barbieri, D. Van Neck, W.H. Dickhoff, Phys. Rev. A 76, 052503 (2007)



The End

Questions?

