SELF-CONSISTENT RPA

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Self-Consistent RPA

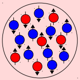
CONTENT

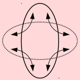
Random Phase Approximation from the Nuclear Physics Point of View

The nucleus is a SELFBOUND system of FOUR different fermions:

neutrons, spin up/down—–-protons, spin up/down

Ground state: HARTREE-FOCK
Mean-Field
relativistic and non-relativistic





Excited states: QUADRUPOLE DEFORMATIONS, BREATHING (COMPRESSION) MODE, etc. $\rightarrow$

TIME DEPENDENT HF

Definitions:
Hamiltonian with two body interaction

$$H = \sum_{\alpha} a^{+}_{\alpha} a_{\alpha} + \frac{1}{4} \sum_{\alpha\beta\gamma\delta} \bar{v}_{\alpha\beta\gamma\delta} a^{+}_{\alpha} a^{+}_{\beta} a_{\delta} a_{\gamma}$$

Density Matrices

$$\rho_{\alpha\alpha'} = \langle \Psi | a^{+}_{\alpha'} a_{\alpha} | \Psi \rangle; \qquad \rho_{\alpha\beta\alpha'\beta'} = \langle \Psi | a^{+}_{\alpha'} a^{+}_{\beta'} a_{\alpha} a_{\alpha} | \Psi \rangle; \qquad \text{ect.}$$

BBGKY hirarchy:

One body density matrix ρ_1

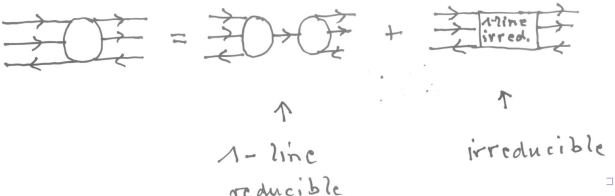
$$i\dot{\rho}_1 = [\rho_1, H] = F_1[\rho_1, \rho_2] \qquad \rightarrow$$

Eq. of Motion for two-body density matrix

$$i\dot{\rho}_2 = [\rho_2, H] = F_2[\rho_2, \rho_3]$$

and so on. We decouple in approximating ρ_3 by $\rho_3 \simeq \rho_2 \otimes \rho_2$

The time ordering in ρ_3 is so that it leads to 2p-1h or 2h-1p correlation functions. It is shown in the figure.



Linearisation:

$$\rho_1 = \rho_1^0 + \delta\rho_1$$

$$C_2 = C_2^0 + \delta C_2 \quad ; \qquad C_2 = \rho_2 - [\rho_1\rho_1]_{a.s.}$$

With the identifications

$$\delta\rho_1 \equiv \chi$$

and

$$\delta C_2 \equiv \mathcal{X}$$

one arrives at the following eigen value problem called
ESRPA (Extended Second RPA)

$$\begin{pmatrix} \mathcal{S} & \mathcal{C} \\ \mathcal{C}^{+} & \mathcal{D} \end{pmatrix} \begin{pmatrix} \chi_1 \\ \mathcal{X}_2 \end{pmatrix} = E \begin{pmatrix} \mathcal{N}_1 & \mathcal{T} \\ \mathcal{T}^{+} & \mathcal{N}_2 \end{pmatrix} \begin{pmatrix} \chi_1 \\ \mathcal{X}_2 \end{pmatrix} \tag{1}$$

with

$$\mathcal{S}_{\alpha\beta\alpha'\beta'} = \langle 0|[a_\beta^{+} a_\alpha, [H, a_{\alpha'}^{+} a_{\beta'}]]|0\rangle = F[\rho, C_2]$$

and

$$\mathcal{N}_{1;\alpha\beta\alpha'\beta'} = n_\beta \delta_{\beta\beta'} - n_\alpha \delta_{\alpha\alpha'}$$

with $n_\alpha = \langle 0|a_\alpha^{+} a_\alpha|0\rangle$ the occupation numbers, etc.

The above one body part is called SELF-CONSISTENT RPA $(C_2 \rightarrow \chi\chi\ )$

$$\mathcal{S}\chi_1 = E\mathcal{N}_1\chi_1$$

Equivalent Green's function formulation

$$G_2^{\omega} = G_2^{(0),\omega} + G_2^{(0),\omega}[M_1^{\text{SCRPA}} + M_2^{\omega}]G_2^{\omega}$$

This is exact formulation of 2-body propagator with kernel dependent only on ONE energy. Neglecting M_2 is equivalent to SCRPA. [NPA 628 (1998)17].

$$M_1 \leftrightarrow \mathcal{S}$$

Relation to Couple Cluster Theory (CCT) wave function

$$|Z\rangle = e^{\frac{1}{4}\sum z_{p_1 p_2 h_1 h_2} J^+_{p_1 h_1} J^+_{p_2 h_2}} |\mathrm{HF}\rangle \quad ; \quad J^+_{ph} = a^+_p a_h$$

One can show

$$Q|Z\rangle = 0$$

with

$$\begin{aligned} Q^+_\nu &= \sum_{ph} [X^\nu_{ph} J^+_{ph} - Y^\nu_{ph} J^-_{ph} \\ &+ \frac{1}{2} \sum_{php_1p_2} \eta_{p_1 p_2 ph} J^0_{p_1 p_2} J^+_{ph} - \frac{1}{2} \sum_{phh_1h_2} \eta_{h_1 h_2 ph} J^0_{h_1 h_2} J^+_{ph} \end{aligned} \qquad (2)$$

and

$$J^- = [J^+]^+ \quad ; \quad J^0_{k_1 k_2} = a^+_{k_2} a_{k_1}$$

$$z = Y/X \quad ; \quad \eta = Xz$$

The non-linear operator is difficult to handle. Therefore, APPROXIMATION

$$J^0_{k_1 k_2} \to \langle J^0_{k_1 k_1} \rangle \delta_{k_1 k_2} \equiv n_{k_1} \delta_{k_1 k_2}$$

Then, we have HFB ansatz for Fermion pairs

$$Q_\nu^+ = \sum_{k>k'} [X_{kk'}^\nu a_k^+ a_{k'} - Y_{kk'}^\nu a_{k'}^+ a_k]$$

Please note that there are also *pp* and *hh* type of apmlitudes. This ansatz solves, e.g., the Tomonaga-Luttinger model exactly.

IMPORTANT PROPERTY:
All nice properties of standard RPA are maintained with SCRPA and also with ESRPA !
Conservation laws, sum-rules, Goldstone mode, Wardidentities.
Kadanoff-Baym ϕ derivable approach has also this property. But numerically untractable!
Resummation of parquet diagrams !

Approximation

$$J^0_{k_1 k_2} \to n_{k_1} \delta_{k_1,k_2} \quad ; \qquad n_k = \langle a^+_{k_1} a_{k_1} \rangle$$

Leads to renormalised Y-amplitude. Very good approximation
SCRPA, variation of sum rule

$$E_\nu = \frac{\langle [Q_\nu, [H, Q^+_\nu]] \rangle}{\langle [Q_\nu, Q^+_\nu] \rangle}$$

This leads to

$$\begin{pmatrix} A[XY] & B[XY] \\ -B^* & -A^* \end{pmatrix} \begin{pmatrix} X \\ Y \end{pmatrix} = \Omega \begin{pmatrix} X \\ Y \end{pmatrix} \tag{3}$$

This is like HFB for bosons, only bosons have been replaced by fermion pairs.
Refs.: Eur. Phys. J. B 89:45; PRB 93, 444329; PRC 72,064305

Illustration of what contains SCRPA kernel, that is effective p-h interaction

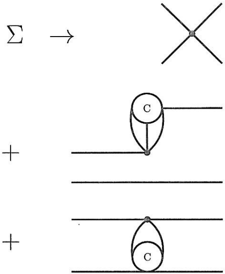


Fig. 8. Schematic representation of the two body mean field. It consists of the direct interaction (full dot), the single particle renormalisation due to two body correlations (C), and screening terms where a two body correlation is echanged between the two lines. It should be mentioned that the two body renormalisations occur instantaneously as indicated when the time runs from left to right. Also symmetric terms should be added interchanging upper and lower lines. The tad-pole graphs are supposed to be included in the single particle lines.

Screening!

Not all is perfect though!

For finite systems transition to symmetry broken state is not continuous; shows wrong first order phase transition.

PRC 72, 064305

SELF-CONSISTENT RANDOM PHASE APPROXIMATION . . .

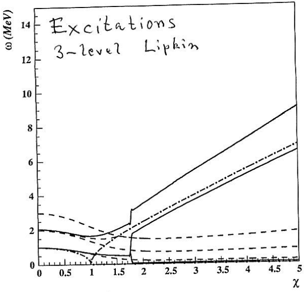


FIG. 7. SCRPA excitation energies vs χ for $N = 20$, $\Delta\epsilon = 0.001$ MeV (full line). Dashed lines give the lowest exact eigenvalues; dot-dashed lines, standard RPA energies. After the phase transition point $\chi = 1$ (standard RPA) and $\chi \approx 2.1$ (SCRPA), a Goldstone mode at zero energy appears.

Henderson et. al PRC 89, 0543

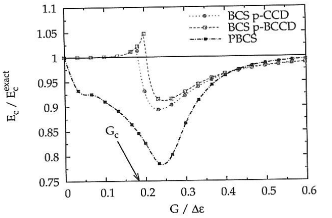


FIG. 2. Fraction of correlation energy recovered in the half-filled pairing Hamiltonian with 100 levels. BCS p-CCD and BCS p-BCCD refer to p-CCD based on a BCS or on a BCS-Brueckner reference, respectively.

Correlation energy, pairing mo

Application to Lipkin model

For simplicity, we consider two level Lipkin model ——— 1

-

——— 0

$$H = \varepsilon J_0 - \frac{V}{2}(J_+ J_+ + J_- J_-)$$

with $[J_-, J_+] = -2J_0$, $[J_0, J_\pm] =_\pm$ and

$$J_0 = \frac{1}{2}\sum_m (c^\dagger_{1m} c_{1m} - c^\dagger_{0m} c_{0m}) \quad J_+ = \sum_m c^\dagger_{1m} c_{0m} \quad J_- = (J_+)^\dagger$$

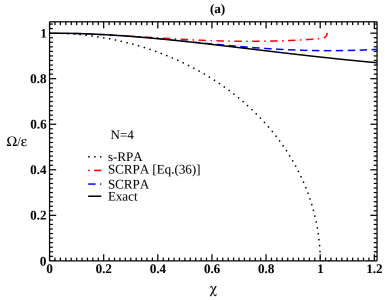
We try exponential with two body operator:

$$|z\rangle = e^{z J_+ J_+} |\mathrm{HF}\rangle$$

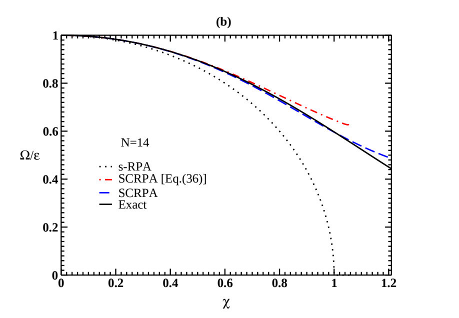
Using following operator with $z = \frac{1}{N}\frac{Y}{X}$ and $\eta = \frac{2}{N}\frac{Y}{X}$

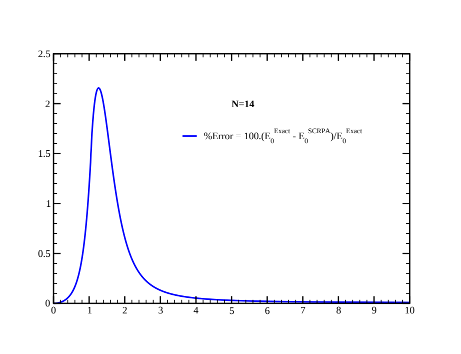
$$Q^\dagger = X J_+ - Y J_- + \eta J_- J_0 \quad \text{we have} \rightarrow \qquad Q|\mathrm{RPA}\rangle = 0!!$$

Again: $J_- J_0 \rightarrow J_- \langle J_0 \rangle$
Scheme can be and has been worked out for general many body problem. Two particle case exact without η term !.

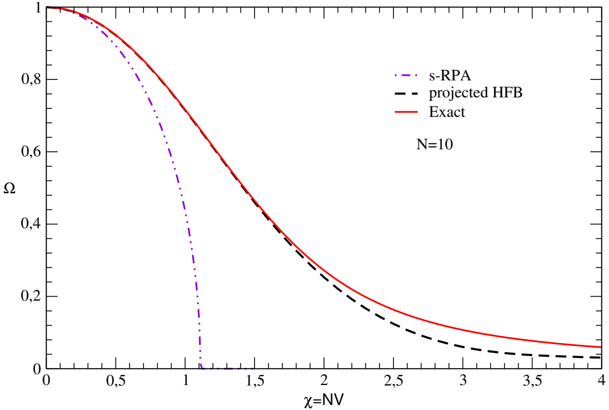


$$\chi = V(N-1)/\varepsilon$$


(b)
N=14
s-RPA
SCRPA [Eq.(36)]
SCRPA
Exact
Ω/ε
χ
0
0.2
0.4
0.6
0.8
1
1.2


N=14
%Error = 100.(E0Exact - E0SCRPA)/E0Exact
0
0.5
1
1.5
2
2.5
3
4
5
6
7
8
9
10

Projected symmetry-broken HFB



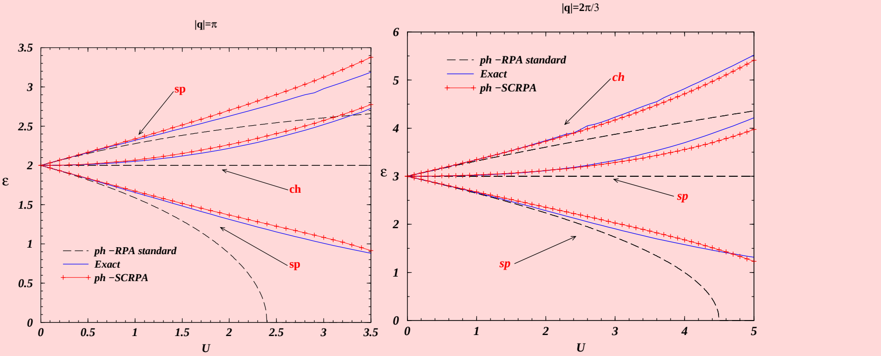
In Lipkin model states become pairwise degenerate!

The HUBBARD Model

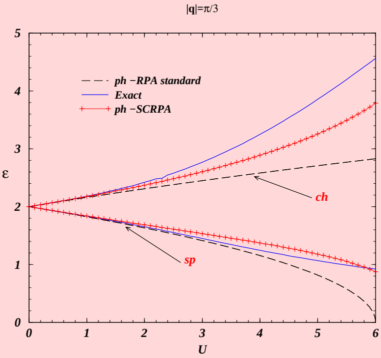
We treat a ring with 6 sites and half filling, i.e. 6 electrons.

$$H = -t \sum_{\langle ij \rangle \sigma} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} \hat{n}_{i+} \hat{n}_{i-} \ , \quad \hat{n}_{i\sigma} = c^{\dagger}_{i\sigma} c_{i\sigma} \tag{4}$$

Two site problem again exact in SCRPA!

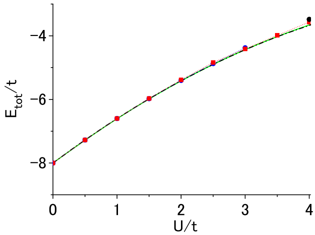


|q|=π
ε
U
sp
ch
sp
ph −RPA standard
Exact
ph −SCRPA
|q|=2π/3
ε
U
ph −RPA standard
Exact
ph −SCRPA
ch
sp
sp



|q|=π/3
ph −RPA standard
Exact
ph −SCRPA
ch
sp
ε
U
0
1
2
3
4
5
6

ground state energy with full TDDM



Goes far beyond instability point $U/t \sim 2.5$

SCRPA in the particle-particle (hole-hole) channel. The pairing or Picket Fence Model.

$$H = \sum_{i=1}^{\Omega}(\varepsilon_i - \lambda)N_i - G\sum_{i,j=1}^{\Omega} P_i^\dagger P_j$$

where

$$P_i = c_{\bar{i}}c_i\ , \quad P_i^\dagger = (P_i)^\dagger\ , \quad N_i = c_i^\dagger c_i + c_{\bar{i}}^\dagger c_{\bar{i}}$$

The pp-RPA operator is

$$\mathcal{A}_\mu^\dagger = \sum_p X_p^\mu P_p^\dagger - \sum_h Y_h^\mu P_h^\dagger$$

Self-Consistent mashinerie gives following results. 2 particle case again exact standard RPA: $E \propto \sqrt{1-G}$; SCRPA: $E \propto \sqrt{1+G}$. Screening has changed sign from attraction to repulsion !!

The Picket Fence Model

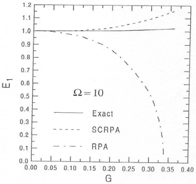
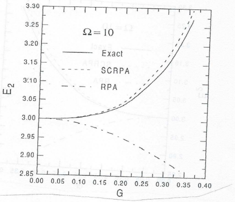


Fig. 3. Groundstate of the system with $\Omega = 10$ and $N = 12$ particles relative to the groundstate of the system with $\Omega = N = 10$.



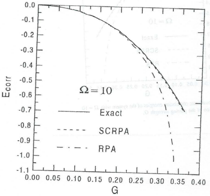


Fig. 1. Groundstate correlation energies of the system with $\Omega = 10$ as a function of the pairing strength G.

Conclusions

i) Decoupling of BBGKY at ρ_2 level: leads to SCRPA

ii) SCRPA conserves all appreciated properties of standard RPA: **Conservation laws, sum-rules, Goldstone mode, gauge invariance, and Ward identities**

iii) Wrong first order transition at break point of symmetry for **finite systems**

iv) Applications: Lipkin model; 1D Hubbard chain; Pairing model. In all cases very good results.