Random Phase Approximation and Extensions

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Jemai, Delion, P.Sch, PRC88(2013)044004

Outline

1. Standard RPA and the quasi boson approximation
2. Improved ground state with Coupled Cluster Theory (CCT)
3. Extension to Self-Consistent RPA (SCRPA); renormalised RPA
4. Some Results
5. Discussion
6. Higher RPA's; odd-particle number RPA; Second RPA
7. Conclusions

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

$$i\frac{d}{dt}\hat{\rho} = [h^{HF}, \hat{\rho}]$$

Small amplitude..........Linear response $\rightarrow$

$$\hat{\rho} = \hat{\rho}_0 + \delta\rho$$

This leads to standard RPA eqs:

$$[\Omega_\nu - (\varepsilon_k - \varepsilon_{k'})]\delta\rho_{k,k'} = (n^0_{k'} - n^0_k)\sum_{l,l'} v_{k,l';k'l}\delta\rho_{l,l'}$$

$$\delta\rho_{ph} \equiv X_{ph} \qquad \delta\rho_{hp} \equiv Y_{ph}$$

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h^{HF} from ENERGY DENSITY FUNCTIONAL (EFFECTIVE FORCES) (about 12 adjustable parameters). Microscopic nucleon- nucleon force unknown !!

Energy Density Functional:

$$\varepsilon(\rho, \tau, \nabla\rho, \tau\rho, \ldots)$$

$$\rho(\mathbf{r}) = \sum_i \phi(\mathbf{r})\phi^*(\mathbf{r}) \qquad \tau(\mathbf{r}) = \sum_i \nabla\phi(\mathbf{r})\nabla\phi^*(\mathbf{r})$$

minimisation with respect to ϕ's $\rightarrow$
HF eqs

$$h^{HF}[\phi_k]\phi_i(\mathbf{r}) = \varepsilon_i\phi_i(\mathbf{r})$$

Vibrations around HF minimum (RPA):

$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} X^\nu \\ Y^\nu \end{pmatrix} = E_\nu \begin{pmatrix} X^\nu \\ -Y^\nu \end{pmatrix}$$

with $A_{ph;p'h'} = \dfrac{\delta^2 \varepsilon}{\delta \rho_{ph} \delta \rho_{p'h'}}$ and $B_{ph;p'h'} = \dfrac{\delta^2 \varepsilon}{\delta \rho_{ph} \delta \rho_{h'p'}}$

GROUND STATE ENERGY:

$$E_0 = E^{HF} + \sum_\nu \sum_{ph} E_\nu |Y^\nu_{ph}|^2$$

- (Applications by other speakers)

Some appreciated properties of RPA

HF: always some symmetries are broken!

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1) Translational Invariance
2) Rotational Invariance
3) Particle Number (BCS)

etc.

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HF-RPA: Goldstone mode at $E_\nu = 0$ (Spurious mode)

Translation: $\frac{P^2}{2Am} = E_{kin}^{total}$

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Conservation laws, Ward Identities fullfilled!!

Sum rule, etc.

Very well established scheme in nuclear physics!

EXTENSIONS OF RPA THEORY.

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SELFCONSISTENT-RPA

-
also
renormalised RPA

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standard RPA $\rightarrow$ Quasi boson approximation $\rightarrow$

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First: ideal bosons $\rightarrow$

Reminder: HFB theory for fermions

BCS ground state

$$|\mathrm{BCS}\rangle = \Pi_k (u_k + v_k a_k^+ a_{\bar{k}}^+)|\mathrm{vac}\rangle \propto e^{\sum_k \frac{v_k}{u_k} a_k^+ a_{\bar{k}}^+}|\mathrm{vac}\rangle$$

quasi-particles:

$$\alpha_k^+ = u_k a_k^+ - v_k a_{\bar{k}}$$

Then, we have the 'killing' property

$$\alpha_k |\mathrm{BCS}\rangle = 0.$$

The u, v coefficients can be determined from minimisation of a sum-rule

$$E_k = \frac{\langle\{\alpha_k, [H, \alpha_k^+]\}\rangle}{\langle\{\alpha_k, \alpha_k^+\}\rangle}; \qquad \{.., ..\} = \text{anticommutator}$$

The minimisation leads to standard BCS eqs

$$\begin{pmatrix} h & \Delta \\ \Delta^+ & -h^* \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix} = E \begin{pmatrix} u \\ v \end{pmatrix},$$

Hartree-Fock Bogoliubov theory for bosons

The Bogoliubov unitary transformation for bosons is

$$q^\dagger_\nu = \sum_\alpha \left[U_{\nu\alpha} b^\dagger_\alpha - V_{\nu\alpha} b_\alpha\right] \quad \leftrightarrow \quad [\, b^\dagger_\alpha = \sum_\nu [U_{\alpha\nu} q^\dagger_\nu + V_{\alpha\nu} q_\nu] \, .$$

where the coefficients U and V are determined by minimisation of

$$e_\nu = \frac{\langle 0|[q_\nu,[H,q^\dagger_\nu]]|0\rangle}{\langle 0|[q_\nu,q^\dagger_\nu]|0\rangle} \; ; \qquad H = \sum t b^\dagger b + \sum v b^\dagger b^\dagger b b$$

$$|0\rangle \equiv |\mathrm{HFB}\rangle \qquad q_\nu|\mathrm{HFB}\rangle = 0 \, , \qquad |\mathrm{HFB}\rangle = e^{\sum \frac{V}{U} b^\dagger b^\dagger} |vac\rangle$$

The minimisation leads to the following set of equations

$$\begin{pmatrix} h[U,V] & \Delta[U,V] \\ \Delta^*[U,V] & h^*[U,V] \end{pmatrix} \begin{pmatrix} U \\ V \end{pmatrix} = E \begin{pmatrix} U \\ -V \end{pmatrix} \, ,$$

with

$$h[U,V] = \langle 0|[b,[H,b^\dagger]]|0\rangle \; ; \qquad \Delta[U,V] = g\langle 0|bb|0\rangle = gUV \, . \qquad (1)$$

$$= \langle 0|[b,[H,b]]|0\rangle \, .$$

SCRPA for particle-hole excitations

RPA excitation operator in the particle-hole channel is

$$Q^\dagger_\nu = \sum_{ph} \left[X^\nu_{ph} A^\dagger_{ph} - Y^\nu_{ph} A_{ph} \right] \ ,$$

$$A^\dagger_{ph} = \sum_\nu [X^\nu_{ph} Q^\dagger_\nu + Y^\nu_{ph} Q_\nu]$$

$$A^\dagger_{ph} = a^\dagger_p a_h \quad \sim B^\dagger_{ph} \quad Q^+_B = XB^+ - YB$$

where $a^\dagger, a$ are fermion creation/destruction operators.

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It is like Bogoliubov **unitary** transformation for ph pairs!

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The operator should have the properties

$$Q^\dagger_\nu |\mathrm{RPA}\rangle = |\nu\rangle \ , \quad Q_\nu |\mathrm{RPA}\rangle = 0 \ . \quad |\mathrm{RPA}\rangle_B \sim e^{\sum z_{p_1 p_2 h_1 h_2} B^+_{p_1 h_1} B^+_{p_2 h_2}} |\mathrm{HF})$$

$$Q_B |\mathrm{RPA}\rangle = 0$$

Evidence of quasi-boson approximation from response fct

$$(\omega - e_k + e_q)R_{kq,k'q'} = \frac{n_q^0 - n_k^0}{\omega - e_k + e_q}[\delta_{kk'}\delta_{qq'} + \sum_{k_1 q_1} \bar{v}_{kq_1 qk_1} R_{k_1 q_1 k' q'}]$$

with

$$R^{t-t'}_{kq,k'q'} = -i\langle T(a_k^+ a_q)_t (a_{q'}^+ a_{k'})_{t'}\rangle$$
$$= -i\Theta(t-t')\langle(a_k^+ a_q)_t (a_{q'}^+ a_{k'})_{t'}\rangle - i\Theta(t'-t)\langle(a_{q'}^+ a_{k'})_{t'} (a_k^+ a_q)_t\rangle$$

Equation of motion

$$(i\frac{\partial}{\partial t} - e_k + e_q)R^{t-t'}_{kq,k'q'} = \delta(t-t')\langle[(a_k^+ a_q), a_{q'}^+ a_{k'}]\rangle + ...$$

Then

$$\langle[(a_k^+ a_q), a_{q'}^+ a_{k'}]\rangle = (n_q - n_k)\delta_{kk'}\delta_{qq'}$$

with $n_k = \langle a_k^+ a_k\rangle \sim n_k^0 = 1$ or $0.$ This is quasi-boson approximation!

Existence of RPA Vacuum

$$|0\rangle \equiv |Z^{(2)}\rangle = e^{Z^{(2)}}|HF\rangle; \quad Z^{(2)} = \frac{1}{4}\sum z^{(2)}_{p_1p_2h_1h_2} A^{\dagger}_{p_1h_1} A^{\dagger}_{p_2h_2}; \quad Q_\nu|Z^{(2)}\rangle = 0 \quad ??$$

$$Q_\nu = \sum_{ph}\left[X^{\nu}_{ph} a^{\dagger}_{h} a_p - Y^{\nu}_{ph} a^{\dagger}_{p} a_h\right]$$

$$+\frac{1}{2}\sum_{php_1p_2} \eta^{\nu}_{p_1pp_2h} a^{+}_{p_2} a_{p_1} a^{+}_{p} a_h - \frac{1}{2}\sum_{phh_1h_2} \eta^{\nu}_{ph_1hh_2} a^{\dagger}_{h_1} a_{h_2} a^{\dagger}_{p} a_h$$

with

$$Y^{\nu}_{ph} = \sum_{p_1h_1} X^{\nu}_{p_1h_1} z^{(2)}_{p_1ph_1h}, \qquad z_{pp'hh'} = \sum_{\nu} (X^{-1})^{\nu}_{ph} Y^{\nu}_{p'h'} \qquad (2)$$

and

$$\eta^{\nu}_{p_1pp_2h} = \sum_{h_1} X^{\nu}_{p_1h_1} z^{(2)}_{pp_2hh_1}, \quad \eta^{\nu}_{ph_1hh_2} = \sum_{p_1} X^{\nu}_{p_1h_1} z^{(2)}_{pp_1hh_2}. \qquad (3)$$

Approximation: $a^{+}_{p_2} a_{p_1} a^{+}_{p} a_h \rightarrow \langle a^{+}_{p_2} a_{p_1}\rangle a^{+}_{p} a_h$, etc.

In order to determine the amplitudes X, Y of (11) we define a generalised sum rule

$$\Omega_\nu = \frac{1}{2}\frac{\langle 0|[Q_\nu,[H,Q_\nu^\dagger]]|0\rangle}{\langle 0|[Q_\nu,Q_\nu^\dagger]|0\rangle} \ .$$

$$= \frac{1}{\langle 0|[Q_\nu,Q_\nu^\dagger]|0\rangle}\sum_\mu (E_\mu - E_0)|\langle 0|Q_\nu|\mu\rangle|^2$$

which we minimise with respect to X, Y.
This leads to the RPA-type of equations of the form

$$\begin{pmatrix} \mathcal{A}_{k_1k_2k_1'k_2'} & \mathcal{B}_{k_1k_2k_1'k_2'} \\ \mathcal{B}^*_{k_1k_2k_1'k_2'} & \mathcal{A}^*_{k_1k_2k_1'k_2'} \end{pmatrix} \begin{pmatrix} X^\nu_{k_1'k_2'} \\ Y^\nu_{k_1'k_2'} \end{pmatrix} = \Omega_\nu \begin{pmatrix} X^\nu_{k_1k_2} \\ -Y^\nu_{k_1k_2} \end{pmatrix} \ ,$$

where

$$\mathcal{A}_{k_1k_2k_1'k_2'} = \langle 0| \left[\delta Q_{k_1k_2}\left[H,\delta Q^\dagger_{k_1'k_2'}\right]\right]|0\rangle \ ,$$

and

$$\mathcal{B}_{k_1k_2k_1'k_2'} = -\langle 0| \left[\delta Q^\dagger_{k_1k_2}\left[H,\delta Q^\dagger_{k_1'k_2'}\right]\right]|0\rangle \ .$$

where

$$\delta Q^\dagger_{k_1k_2} = \frac{A_{k_1k_2}}{\sqrt{n_{k_2}-n_{k_1}}} \; , \quad A_{k_1k_2} = a^\dagger_{k_1} a_{k_2} \; ,$$

are the normalised pair creation operators and

$$n_k = \langle 0 | a^\dagger_k a_k | 0 \rangle \; ,$$

are the single particle occupation numbers
The Bogoliubov orthonormality relations allow us to invert the operator (14)

$$\frac{A^\dagger_{k_1k_2}}{\sqrt{n_{k_2}-n_{k_1}}} = \sum_\nu \left(X^{\nu *}_{k_1k_2} Q^\dagger_\nu + Y^{\nu *}_{k_1k_2} Q_\nu \right) \; .$$

The double commutators in $\mathcal{A}, \mathcal{B}$ contain the occupation numbers n_k and $\langle A^\dagger A \rangle$ or $\langle AA \rangle$. The latter can be expressed by X, Y amplitudes via killing relation $Q|\mathrm{RPA}\rangle = 0$.

$$\langle A^\dagger A \rangle = F[X, Y] \qquad \langle AA \rangle = G[X, Y]$$

With inversion and killing condition, we get with CC wave fct

$$n_k = n_k[X, Y]$$

and thus

$$\begin{pmatrix} \mathcal{A}[X, Y] & \mathcal{B}[X, Y] \\ \mathcal{B}^*[X, Y] & \mathcal{A}^*[X, Y] \end{pmatrix} \begin{pmatrix} X \\ Y \end{pmatrix} = E \begin{pmatrix} X \\ -Y \end{pmatrix}$$

Leads to a fully Self-consistent scheme, very similar to HFB eqs for bosons.
Here, HFB for fermion pairs.
Linearising with $X \to 1$, $Y \to 0$ in matrix $\to$ standard RPA.

Determination of optimal single particle basis

Minimisation of ground state energy with respect to s.p. basis $\rightarrow$

$$\langle [H, Q^\dagger] \rangle = \langle [H, a_k^\dagger a_{k'}] \rangle = \Psi[X, Y; \phi] = 0$$

Very natural result, since just another Equation of Motion! Again only n_k and $\langle AA \rangle$ enter and, thus, s.p. basis gets coupled to X, Y amplitudes, selfconsistently.

Application to Lipkin model

For simplicity, we consider two level Lipkin model

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——— 1

——— 0

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

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

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

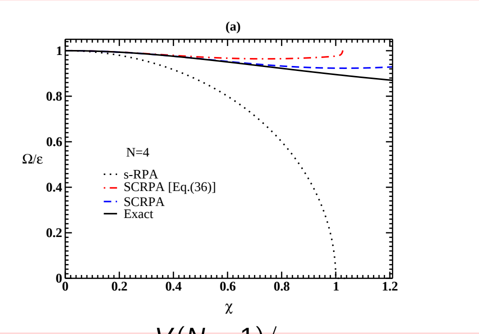
We try exponential with two body operator:

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

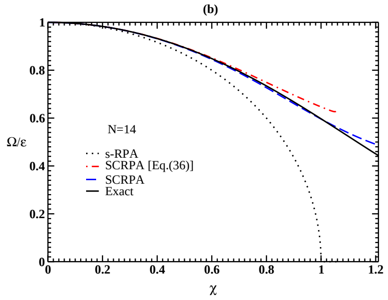
Using following operator with $z = \frac{1}{N}\frac{Y}{X}$ and $\eta = \frac{2}{N}\frac{Y}{X}$

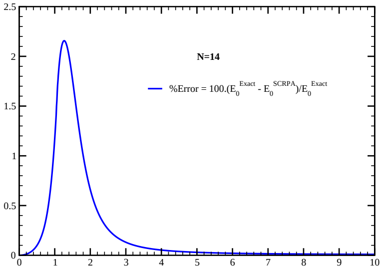
$$Q^\dagger = XJ_+ - YJ_- + \eta J_-J_0 \quad \text{we have} \rightarrow \qquad Q|\mathrm{RPA}\rangle = 0!!$$

Again: $J_- J_0 \to J_- \langle J_0 \rangle$
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

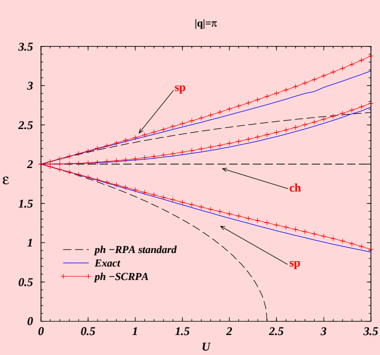
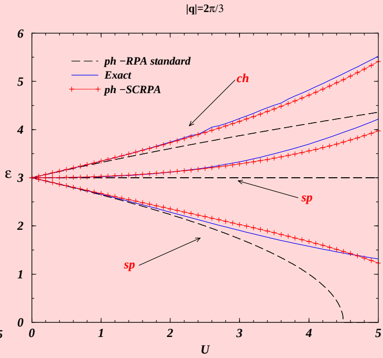

N=14
%Error = 100.(E0 Exact - E0 SCRPA)/E0 Exact

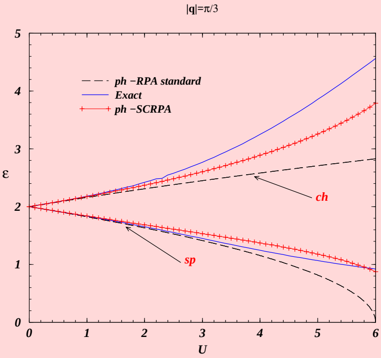
The HUBBARD Model

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

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

Two site problem again exact in SCRPA!


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

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



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

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: $E \propto \sqrt{1+G}$ (exact(!)). Screening has changed sign from attraction to repulsion !!

The Picket Fence Model

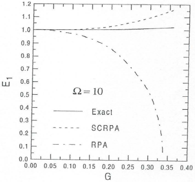
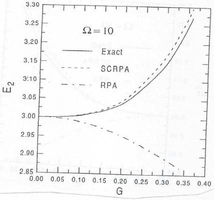


Fig. 3. Groundstate of the system with $\Omega = 10$ and $N = 12$ particles relative to the groundstate of the system with $\Omega = N = 10$.



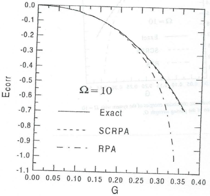


Fig. 1. Groundstate correlation energies of the system with $\Omega = 10$ as a function of the pairing strength G.

Estimate of violation of Pauli principle

$$\sum_{pp'} \langle M_p M_{p'} \rangle = \sum_{ph} \langle M_h M_p \rangle$$

$$M_p = c_p^+ c_p + c_{\bar{p}}^+ c_{\bar{p}}; \text{etc.}$$

Above sumrule is violated by about 4 percent.

DISCUSSION

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Killing condition in SCRPA nearly fullfilled. Then theory nearly Raleigh-Ritz variational. In all models two particle case exact.
Pleasent properties of RPA remain fullfilled: Goldstone mode appears $\rightarrow$ Delion
This is a very strong property!! Difficult to obtain with other approaches.
Sum rules satisfied!
Can be formulated with Green's functions and at finite temperature.
An approximation to SCRPA $\rightarrow$ renormalised RPA:
In standard RPA one only replaces

$$n_k^0 \rightarrow n_k = n_k[X, Y]$$

Yields often appreciable improvement over standard RPA; much easier than SCRPA. (F. Catara et al., PLB 306(1993)197; PRB 51(1995)4569)
So far some problems in 'deformed' region: transition from 'spherical' to deformed region is discontinuous like a first order phase transition what should not be. Further work is in progress on this problem. It seems that same problem appears with CCT (Dukelsky)

CONCLUSIONS

SCRPA has quite satisfying properties. Realistic applications to nuclear shell model and comparison with large scale shell model calculations are in progress.

RPA for odd particle number systems

It is interesting that our vacuum state $|Z\rangle$ is also the vacuum to an odd number RPA operator (for calculating $N \pm 1$ systems)

$$q_{a,\mu}|Z\rangle = q_{r,\mu}|Z\rangle = 0$$

with

$$q^\dagger_{a,\mu} = \sum_p y^\mu_p a^\dagger_p - \frac{1}{2}\sum_{hh'p} Y^\mu_{hh':p} a^\dagger_h a^\dagger_{h'} a_p \quad q^\dagger_{r,\mu} = \sum_h y^\mu_h a_h - \frac{1}{2}\sum_{pp':h} Y^\mu_{pp':h} a^\dagger_h a_p a_{p'}$$

under the condition

$$\sum_p y^\mu_p z_{pp'hh'} = Y^\mu_{hh':p'}\ , \quad \sum_h y^\mu_h z_{pp'hh'} = Y^\mu_{pp':h'}$$

We minimise again energy weighted sum rule for an average single particle energy and obtain

$$\langle Z|\{\delta q,[H,q^\dagger]\}\rangle = e\langle Z|\{\delta q,q^\dagger\}|Z\rangle$$

Double commutator leads to three particle correlation fct. Factorisation into products of s.p. and two particle correlation fcts preserves the property that two particle system stays exact. This may be a good approximation in general. Two body correlation fct can be evaluated by SCRPA as before. Should give quite reasonable results.

Conclusions

Instead of evaluating RPA eqs with HF we evaluate it with $|Z\rangle$ (CCT).

We obtain naturally a fully selfconsistent RPA scheme in X, Y amplitudes.

Results in non trivial model cases very encouraging!

Extension to odd particle numbers.

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