

Random Phase Approximation and Extensions

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Outline

1. Standard RPA from energy density functional in nuclear physics
2. Extension to Self-Consistent RPA (SCRPA); **renormalised RPA**
3. Some Results
4. Discussion
5. Improved ground state
6. Higher RPA's; **Second RPA**
7. Self Consistent RPA for p-p and h-h excitations
8. 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. →

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:

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

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

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

Energy Density Functional:

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

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

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

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):

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

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

GROUND STATE ENERGY:

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

- (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 fulfilled!!

Sum rule, etc.

Very well established scheme in nuclear physics!

EXTENSIONS OF RPA THEORY.

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SELFCONSISTENT-RPA

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also

renormalised RPA

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standard RPA \rightarrow Quasi boson approximation \rightarrow

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First: ideal bosons \rightarrow

Hartree-Fock Bogoliubov theory for bosons

The Bogoliubov **unitary** transformation for bosons is

$$q_\nu^\dagger = \sum_\alpha [U_{\nu\alpha} b_\alpha^\dagger - V_{\nu\alpha} b_\alpha] \quad \leftrightarrow \quad [b_\alpha^\dagger = \sum_\nu [U_{\alpha\nu} q_\nu^\dagger + V_{\alpha\nu} q_\nu].$$

where the coefficients U and V are determined by minimisation of

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

$$|0\rangle \equiv |\text{HFB}\rangle \quad q_\nu |\text{HFB}\rangle = 0$$

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

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

SCRPA for particle-hole excitations

RPA excitation operator in the particle-hole channel is

$$Q_{\nu}^{\dagger} = \sum_{ph} \left[X_{ph}^{\nu} A_{ph}^{\dagger} - Y_{ph}^{\nu} A_{ph} \right] ,$$

$$A_{ph}^{\dagger} = c_{ph} \sum_{\nu} \left[X_{ph}^{\nu} Q_{\nu}^{\dagger} + Y_{ph}^{\nu} Q_{\nu} \right]$$

$$A_{ph}^{\dagger} = a_p^{\dagger} a_h$$

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

$$Q_{\nu}^{\dagger} |RPA\rangle = |\nu\rangle , \quad Q_{\nu} |RPA\rangle = 0 .$$

In order to determine the amplitudes X, Y of (10) we define a generalised sum rule

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

which we minimise with respect to X, Y .

This leads to the RPA-type of equations of the form

$$\begin{pmatrix} \mathcal{A}_{k_1 k_2 k'_1 k'_2} & \mathcal{B}_{k_1 k_2 k'_1 k'_2} \\ \mathcal{B}_{k_1 k_2 k'_1 k'_2}^* & \mathcal{A}_{k_1 k_2 k'_1 k'_2}^* \end{pmatrix} \begin{pmatrix} X_{k'_1 k'_2}^\nu \\ Y_{k'_1 k'_2}^\nu \end{pmatrix} = \Omega_\nu \begin{pmatrix} X_{k_1 k_2}^\nu \\ -Y_{k_1 k_2}^\nu \end{pmatrix},$$

where

$$\mathcal{A}_{k_1 k_2 k'_1 k'_2} = \langle 0 | \left[\delta Q_{k_1 k_2}, \left[H, \delta Q_{k'_1 k'_2}^\dagger \right] \right] | 0 \rangle,$$

and

$$\mathcal{B}_{k_1 k_2 k'_1 k'_2} = -\langle 0 | \left[\delta Q_{k_1 k_2}^\dagger, \left[H, \delta Q_{k'_1 k'_2}^\dagger \right] \right] | 0 \rangle.$$

where

$$\delta Q_{k_1 k_2}^\dagger = \frac{A_{k_1 k_2}}{\sqrt{n_{k_2} - n_{k_1}}}, \quad A_{k_1 k_2} = a_{k_1}^\dagger a_{k_2},$$

are the normalised pair creation operators and

$$n_k = \langle 0 | a_k^\dagger a_k | 0 \rangle,$$

are the single particle occupation numbers

The Bogoliubov orthonormality relations allow us to invert the operator (14)

$$\frac{A_{k_1 k_2}^\dagger}{\sqrt{n_{k_2} - n_{k_1}}} = \sum_{\nu} (X_{k_1 k_2}^{\nu*} Q_{\nu}^\dagger + Y_{k_1 k_2}^{\nu*} Q_{\nu}).$$

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

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

Occupation numbers can be expanded

$$a_k^\dagger a_k = [A^\dagger A + c_2 A^\dagger A^\dagger A A + \dots]_k$$

With inversion and killing condition, we get

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

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.
Linearising with $X \rightarrow 1$, $Y \rightarrow 0$ in matrix \rightarrow **standard RPA**.

Determination of **optimal single particle basis**

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

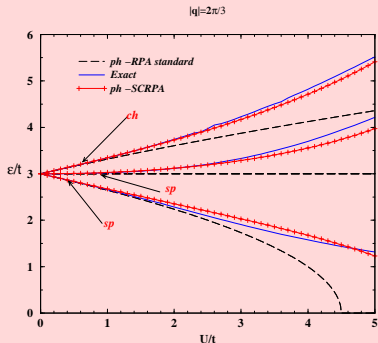
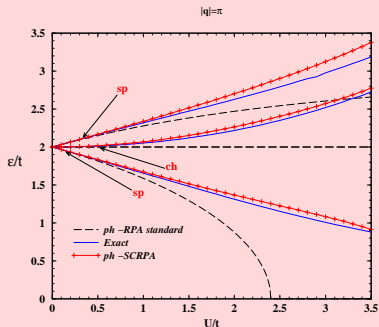
$$\langle [H, Q^\dagger] \rangle = \langle [H, a_k^\dagger a_{k'}] \rangle = \Psi[X, Y; \phi] = 0$$

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.

SOME RESULTS: Hubbard model; periodic linear chain, six sites,



half- filling



M. Jemai et al., PRB 71(2005)085115

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Two site case: EXACT SOLUTION !

DISCUSSION

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PROBLEM: Has killing condition $Q|RPA \rangle = 0$ a solution? (Linderberg-Oehrn, Toyoda, ..)

Otherwise: **Approximate decoupling scheme**

Pleasant properties of RPA remain fulfilled: Goldstone mode appears →
Delion

This is a very strong property!! Difficult to obtain with other approaches.
Sum rules satisfied!

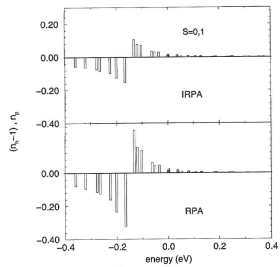
Can be formulated with Green's functions and at finite temperature. (talk by
Dinh Dang; A. Storozhenko et al., Annals Phys. 307(2003)308

An approximation to SCRPA → 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)



Further considerations on 'killing' condition

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

- ———— 0

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

with

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

We try exponential with two body operator:

$$|z\rangle = e^{z J_+ J_+} |\text{HF}\rangle \quad (\text{similar to } \exp[S] \text{ or coupled cluster ansatz}).$$

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

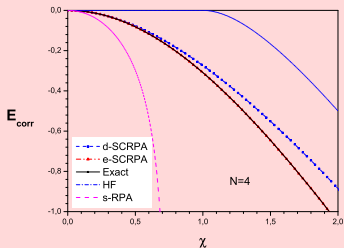
$$Q^\dagger = X J_+ - Y J_- + \frac{2}{N} Y J_- J_0 \quad \text{we have} \rightarrow \quad Q|\text{RPA}\rangle = 0!!$$

Problem with inversion, since nonlinear transformation. But

$$\epsilon = \frac{2}{N} Y = \text{small !}$$

Can be treated perturbatively.

Scheme can be and has been worked out for general many body problem.



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

SECOND RPA; double Goldstone modes

Second RPA attempts to include 2p-2h configurations. We again can start from [Equation of Motion method](#)

$$Q^\dagger = \sum_{k_1 k_2} X_{k_1 k_2} c_{k_1}^\dagger c_{k_2} + \frac{1}{4} \sum_{k_1 k_2 k_3 k_4} X_{k_1 k_2 k_3 k_4} c_{k_1}^\dagger c_{k_1}^\dagger c_{k_3} c_{k_4}$$

and minimise double commutator

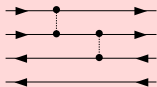
$$\Omega_\nu = \langle 0 | [Q_\nu, [H, Q_\nu^\dagger]] | 0 \rangle / \langle 0 | [Q_\nu, Q_\nu^\dagger] | 0 \rangle .$$

Evaluating expectation values with HF ground state leads to:

$$\begin{aligned} (\omega_\mu - \varepsilon_1 - \varepsilon_2 + \varepsilon_3 + \varepsilon_4) X_{1234}^\mu &= \sum_{1'2'} (1 - n_1^0 - n_2^0) v_{12,1'2'} X_{1'2'34}^\mu \\ &- \sum_{3'4'} (1 - n_3^0 - n_4^0) v_{34,3'4'} X_{123'4'}^\mu \\ &- \sum_{1'3'} (n_3^0 - n_1^0) v_{13',31'} X_{1'23'4}^\mu \\ &+ \sum_{2'4'} (n_4^0 - n_2^0) v_{24',42'} X_{12'34'}^\mu \end{aligned}$$

We see that there are two types of phase space (Pauli blocking) factors:

$$1 - n_1^0 - n_2^0 = (1 - n_1^0)(1 - n_2^0) - n_1^0 n_2^0$$



$$n_2^0 - n_1^0 = (1 - n_1^0)n_2^0 - (1 - n_2^0)n_1^0$$

The first ones are in front of particle-particle matrix elements and the second ones in front of particle-hole ones.

One also sees that to obtain these eqs one only has to augment the TDA Pauli factors by the second terms, ie replace TDA Pauli factors by RPA Pauli factors.

These generalised Second RPA eqs give rise to 9 different amplitudes X_{1234} with all possible types of indices, i.e. $1234 \rightarrow$ pppp, ppph, pphh, phhh, hhhh, hhpp, hphp, hphh, hphh

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M. Tohyama, P. Sch., EPJA19(2004)203

Standard HF-RPA obeys the Goldstone theorem for one body symmetry operator

$$Q^\dagger = \hat{S} = \sum_{kk'} s_{kk'} a_{k'}^\dagger a_k$$

But what about in second RPA with

$$Q^\dagger = \hat{S}\hat{S} ?$$

It can be shown that one needs ALL types of two body amplitudes so that double Goldstone mode appears at zero energy !

Self Consistent RPA for p-p and h-h excitations

The starting point is the definition of the so-called two particle addition operator

$$Q_{\rho}^{\dagger} = \frac{1}{2} \sum_{p_1 p_2} X_{p_1 p_2}^{\rho} a_{p_1}^{\dagger} a_{p_2}^{\dagger} - \frac{1}{2} \sum_{h_1 h_2} Y_{h_1 h_2}^{\rho} a_{h_1}^{\dagger} a_{h_2}^{\dagger}, \quad (2)$$

where p, h again refer to the particle and hole states corresponding to an optimal single particle basis yet to be defined. The X^{ρ}, Y^{ρ} amplitudes can, as before, be determined from the minimisation of the generalised sum rule

$$\Omega_{\rho} = \frac{\langle 0 | [Q_{\rho}, [H, Q_{\rho}^{\dagger}]] | 0 \rangle}{\langle [Q_{\rho}, Q_{\rho}^{\dagger}] \rangle}, \quad (3)$$

which leads to

$$\begin{pmatrix} \mathcal{A} & \mathcal{B} \\ -\mathcal{B} & -\mathcal{C} \end{pmatrix} \begin{pmatrix} X^{\rho} \\ Y^{\rho} \end{pmatrix} = \Omega_{\rho} \begin{pmatrix} X^{\rho} \\ Y^{\rho} \end{pmatrix}, \quad (4)$$

CONCLUSIONS

Equation of Motion Method probably not exploited enough for Many body problems with $D > 1$

Equations are of Schroedinger type and numerically accessible.

Very difficult to implement conservation laws and Ward identities otherwise, e.g. with Φ - derivable functional a la Kadanoff and Baym.

There are unsolved problems but eventually can be overcome.

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COLLABORATORS:

Jorge Dukelsky, Doru Delion, Mitsuru Tohyama, Mohsen Jemai,

The vacuum to the corresponding destruction operator is determined by

$$Q_{\nu}^{\dagger}|0\rangle = |\nu\rangle, \quad (6)$$

with

$$Q_{\nu}|0\rangle = 0. \quad (7)$$

Given that $|0\rangle$ and $|\nu\rangle$ are, respectively, exact ground state and excited states of the many body Hamiltonian, i.e.

$$\begin{aligned} H|\nu\rangle &= E_{\nu}|\nu\rangle \\ H|0\rangle &= E_0|0\rangle, \end{aligned} \quad (8)$$

one can write down such an excitation operator.
With $\langle\nu|0\rangle = 0$ the solution to (6) and (7) is

$$Q_{\nu}^{\dagger} = |\nu\rangle\langle 0|. \quad (9)$$

With the help of the Schrödinger equation we then obtain

$$[H, Q_\nu^\dagger]|0\rangle = \Omega_\nu Q_\nu^\dagger|0\rangle, \quad (10)$$

with $Q_\nu = E_\nu - E_0$ the excitation energy.

Multiplying from the left with an arbitrary variation of the form $\langle 0|\delta Q$ we obtain

$$\langle 0|[\delta Q, [H, Q_\nu^\dagger]]|0\rangle = \Omega_\nu \langle 0|[\delta Q, Q_\nu^\dagger]|0\rangle. \quad (11)$$

The variation $\delta Q^\dagger|0\rangle$ exhausting the complete Hilbert space, (11) is equivalent to minimise the mean excitation energy given by

$$\Omega_\nu = \frac{\langle 0|[Q_\nu, [H, Q_\nu^\dagger]]|0\rangle}{\langle 0|[Q_\nu, Q_\nu^\dagger]|0\rangle}. \quad (12)$$

With the exact operator (9), (12) is equal to exact excitation energy of the state $|\nu\rangle$, i.e. $\Omega_\nu = E_\nu - E_0$.

Self Consistent RPA for p-h excitations

An obvious but important observation is that the creation operator (6) is non hermitian and that it is an N -body operator.

It is therefore a natural idea to develop this operator in a series of one, two, ..., N -body operators as follows

$$\begin{aligned} Q_{\nu}^{\dagger} &= \sum_{k_1 k_2} \chi_{k_1 k_2}^{\nu} a_{k_1}^{\dagger} a_{k_2} \\ &+ \sum_{k_1 k_2 k_3 k_4} \chi_{k_1 k_2 k_3 k_4}^{\nu} a_{k_1}^{\dagger} a_{k_2}^{\dagger} a_{k_3} a_{k_4} + \dots \end{aligned} \tag{13}$$

For the moment we only want to consider the one body part of (13) and only later we will also discuss the two body part.

The one body part only has non hermitian pieces if we choose the amplitudes

$$\chi_{k_1 k_2}^\nu \equiv \tilde{X}_{k_1 k_2}^\nu \text{ with } k_1 > k_2$$

$$\chi_{k_1 k_2}^\nu \equiv -\tilde{Y}_{k_1 k_2}^\nu \text{ with } k_1 < k_2 \text{ and all } X_{kk}^\nu \equiv 0.$$

We then write for the one body part of (13)

$$Q_\nu^\dagger = \sum_{k_1 > k_2} \left[\tilde{X}_{k_1 k_2}^\nu a_{k_1}^\dagger a_{k_2} - \tilde{Y}_{k_1 k_2}^\nu a_{k_2}^\dagger a_{k_1} \right]. \quad (14)$$

It is very important to write down the operator Q_ν^\dagger of (14) in a single particle basis which is optimal.

As usual we will choose the one which minimises the ground state energy.

This single particle basis will be given by a generalised single particle mean field Hamiltonian and we will divide the space into occupied levels (h : holes) and unoccupied levels (p : particles).

Let us consider 4 levels with the Fermi energy in the middle. We then order the states according to this energy $p_4 > p_3 > h_2 > h_1$.

We thus have six X^ν amplitudes:

$$X_{p_4 p_3}^\nu, X_{h_2 h_1}^\nu, X_{p_4 h_2}^\nu, X_{p_4 h_1}^\nu, X_{p_3 h_2}^\nu, X_{p_3 h_1}^\nu.$$

and corresponding six Y^ν amplitudes.

This leads to an excited state $|\nu\rangle = Q_\nu^\dagger|0\rangle$ which is not normalised, i.e.

$$\langle\nu|\nu\rangle = \langle 0|[Q_\nu, Q_\nu^\dagger]|0\rangle \neq 1.$$

We therefore introduced slightly modified amplitudes and write

$$Q_{\nu}^{\dagger} = \sum_{k_1 > k_2} \left(X_{k_1 k_2}^{\nu} \delta Q_{k_1 k_2}^{\dagger} - Y_{k_1 k_2}^{\nu} \delta Q_{k_1 k_2} \right), \quad (15)$$

where

$$\delta Q_{k_1 k_2}^{\dagger} = \frac{A_{k_1 k_2}}{\sqrt{n_{k_2} - n_{k_1}}}, \quad A_{k_1 k_2} = a_{k_1}^{\dagger} a_{k_2}, \quad (16)$$

are the normalised pair creation operators and

$$n_k = \langle 0 | a_k^{\dagger} a_k | 0 \rangle, \quad (17)$$

are the single particle occupation numbers. With this choice one immediately verifies that with

$$\sum_{k_1 > k_2} \left(|X_{k_1 k_2}^{\nu}|^2 - |Y_{k_1 k_2}^{\nu}|^2 \right) = 1, \quad (18)$$

The excited states $|\nu\rangle$ are normalised under the assumption that the single particle density matrix only has diagonal elements that is

$$\rho_{kk'} = \langle 0 | a_k^\dagger a_{k'} | 0 \rangle = n_k \delta_{kk'} , \quad (19)$$

a fact which will become clear in a moment. With this we finally can write for Eq. (11)

$$\begin{pmatrix} \mathcal{A}_{k_1 k_2 k'_1 k'_2} & \mathcal{B}_{k_1 k_2 k'_1 k'_2} \\ -\mathcal{B}_{k_1 k_2 k'_1 k'_2}^* & -\mathcal{A}_{k_1 k_2 k'_1 k'_2}^* \end{pmatrix} \begin{pmatrix} X_{k'_1 k'_2}^\nu \\ Y_{k'_1 k'_2}^\nu \end{pmatrix} = \Omega_\nu \begin{pmatrix} X_{k_1 k_2}^\nu \\ Y_{k_1 k_2}^\nu \end{pmatrix} , \quad (20)$$

where

$$\mathcal{A}_{k_1 k_2 k'_1 k'_2} = \langle 0 | \left[\delta Q_{k_1 k_2} \left[H, \delta Q_{k'_1 k'_2}^\dagger \right] \right] | 0 \rangle , \quad (21)$$

and

$$\mathcal{B}_{k_1 k_2 k'_1 k'_2} = -\langle 0 | \left[\delta Q_{k_1 k_2}^\dagger \left[H, \delta Q_{k'_1 k'_2}^\dagger \right] \right] | 0 \rangle . \quad (22)$$

We realise that (20) has exactly the same mathematical structure as the standard RPA equations. Therefore in this respect all standard RPA properties are preserved.

It is useful to introduce the matrices

$$\mathcal{X} = \begin{pmatrix} X & Y^* \\ Y & X^* \end{pmatrix}, \quad \mathcal{N} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (23)$$

Equation (20) can then be written as

$$\mathcal{S}\mathcal{X} = \mathcal{N}\mathcal{X}\Omega, \quad (24)$$

where

$$\mathcal{S} = \begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix}, \quad (25)$$

and the diagonal matrix Ω contain the eigenvalues

$$\begin{pmatrix} \Omega_\nu \\ -\Omega_\nu \end{pmatrix}, \quad (26)$$

if \mathcal{S} is positive defined.

Simple matrix algebra shows that

$$\begin{aligned} [\Omega, \mathcal{X}^\dagger \mathcal{N} \mathcal{X}] &= (\mathcal{N} \mathcal{X} \Omega)^\dagger \mathcal{X} - \mathcal{X}^\dagger (\mathcal{N} \mathcal{X} \Omega) \\ &= \mathcal{X}^\dagger (\mathcal{S}^\dagger - \mathcal{S}) \mathcal{X} = 0, \end{aligned} \quad (27)$$

that is, Ω commutes with $\mathcal{X}^\dagger \mathcal{N} \mathcal{X}$, and thus $\mathcal{X}^\dagger \mathcal{N} \mathcal{X}$ is diagonal

The normalisation (18) corresponds to the more general orthogonality relations

$$\mathcal{X}^\dagger \mathcal{N} \mathcal{X} = \mathcal{N} . \quad (28)$$

This closure condition is obtained by multiplying (28) with \mathcal{N} , which shows that $\mathcal{N} \mathcal{X} \mathcal{N}$ is the inverse of \mathcal{X}^\dagger , or

$$\mathcal{X} \mathcal{N} \mathcal{X}^\dagger = \mathcal{N} , \quad (29)$$

which gives explicitly

$$\sum_{\nu} \left(X_{k_1 k_2}^{\nu} X_{k'_1 k'_2}^{\nu*} - Y_{k_1 k_2}^{\nu*} Y_{k'_1 k'_2}^{\nu} \right) = \delta_{k_1 k'_1} \delta_{k_2 k'_2} . \quad (30)$$

These orthonormality relations allow us to invert the operator (15)

$$a_{k_1}^\dagger a_{k_2} = \sqrt{n_{k_2} - n_{k_1}} \sum_{\nu} \left(X_{k_1 k_2}^{\nu*} Q_{\nu}^\dagger + Y_{k_1 k_2}^{\nu*} Q_{\nu} \right) . \quad (31)$$

With (7) it then follows that the density matrix $\langle 0 | a_k^\dagger a_{k'} | 0 \rangle$ only has diagonal elements, as postulated earlier.

Hartree-Fock basis

The equations (20) are, however, much more general and it is obvious that, if the expectation values in (20) are evaluated with the RPA ground state $|RPA\rangle$ defined in (7), then the matrices \mathcal{A} and \mathcal{B} will depend in a complicated nonlinear way on the amplitudes X and Y . This we will call the Self-Consistent RPA (SCRPA).

If, instead of closing the EMM from the left with a variation, we project from the left with the ground state, we obtain with (7) obviously the most important equation

$$\langle 0|[H, Q_\nu^\dagger]|0\rangle = \langle 0|[H, Q_\nu]|0\rangle = 0. \quad (32)$$

Because there are as many operators Q_ν^\dagger, Q_ν as there are components $a_{k_1}^\dagger a_{k_2}, a_{k_2}^\dagger a_{k_1}$ we also can write for (32)

$$\langle 0|[H, a_{k_1}^\dagger a_{k_2}]|0\rangle = \langle 0|[H, a_{k_2}^\dagger a_{k_1}]|0\rangle = 0, \quad (33)$$

where we again recall our convention $k_1 > k_2$.

With the RPA ground state the single particle basis becomes coupled to the two body RPA correlations as follows

$$\sum_{m'} H_{mm'} C_{m'\alpha} = \epsilon_{\alpha} n_{\alpha} C_{m\alpha} , \quad (34)$$

where $C_{m\alpha}$ are the transformation coefficients defining the HF basis. We also introduced as short-hand notation

$$\begin{aligned} H_{mm'} &\equiv n_m \sum_{\mu} \epsilon_{\mu} C_{m\mu} C_{m'\mu} \\ &+ \frac{1}{2} \sum_{jkl} \sum_{\mu\beta\gamma\delta} [\langle mjkl \rangle v_{\alpha\beta\gamma\delta} + \langle jmk l \rangle v_{\beta\alpha\gamma\delta} \\ &+ \langle kjml \rangle v_{\gamma\beta\alpha\delta} + \langle ljkm \rangle v_{\delta\beta\gamma\alpha}] C_{m'\mu} C_{j\beta} C_{k\gamma} C_{l\delta} , \end{aligned} \quad (35)$$

where $\langle ijkl \rangle \equiv \langle a_i^{\dagger} a_j a_k^{\dagger} a_l \rangle$ are the two body densities which together with occupation numbers n_m depend on the RPA amplitudes.

Ground state

There exists, however, another rather direct way to close the system of equations. This implies an approximate solution of (7) (remember that (7) only can be solved exactly in very simplified model cases). One namely can show that the following form of the ground state

$$|0\rangle \sim |HF\rangle + \frac{1}{4} \sum_{p_1 p_2 h_1 h_2} z_{p_1 p_2 h_1 h_2} a_{p_1}^\dagger a_{p_2}^\dagger a_{h_2} a_{h_1} |HF\rangle, \quad (36)$$

with

$$z_{p_1 p_2 h_1 h_2} = -z_{p_2 p_1 h_1 h_2} = -z_{p_1 p_2 h_2 h_1} = z_{p_2 p_1 h_2 h_2} \quad (37)$$

and

$$z_{p_1 p_2 h_1 h_2} = \sum_{\nu} Y_{p_1 h_1}^{\nu} (X^{-1})_{p_2 h_2}^{\nu}, \quad (38)$$

is the solution of 7) under the condition that higher $2p - 2h$ excitations are neglected and the Q^\dagger operators are restricted to ph configurations.

Using this ground state, all expectation values can be calculated as functions of X , Y and therefore the SCRPA equations are closed.

Self Consistent RPA for p-p and h-h excitations

The starting point is the definition of the so-called two particle addition operator

$$A_{\rho}^{\dagger} = \frac{1}{2} \sum_{\rho_1 \rho_2} X_{\rho_1 \rho_2}^{\rho} a_{\rho_1}^{\dagger} a_{\rho_2}^{\dagger} - \frac{1}{2} \sum_{h_1 h_2} Y_{h_1 h_2}^{\rho} a_{h_1}^{\dagger} a_{h_2}^{\dagger}, \quad (39)$$

where p, h again refer to the particle and hole states corresponding to an optimal single particle basis yet to be defined. The X^{ρ} , Y^{ρ} amplitudes can, as before, be determined from the minimisation of the generalised sum rule

$$\Omega_{\rho} = \frac{\langle 0 | [A_{\rho}, [H, A_{\rho}^{\dagger}]] | 0 \rangle}{\langle [A_{\rho}, A_{\rho}^{\dagger}] \rangle}, \quad (40)$$

which leads to

$$\begin{pmatrix} \mathcal{A} & \mathcal{B} \\ -\mathcal{B} & -\mathcal{C} \end{pmatrix} \begin{pmatrix} X^{\rho} \\ Y^{\rho} \end{pmatrix} = \Omega_{\rho} \begin{pmatrix} X^{\rho} \\ Y^{\rho} \end{pmatrix}, \quad (41)$$

and

$$\begin{aligned}\delta P_{p_1 p_2}^\dagger &= \frac{a_{p_1}^\dagger a_{p_2}^\dagger}{\sqrt{1 - n_{p_1} - n_{p_2}}} \\ \delta P_{h_1 h_2}^\dagger &= \frac{a_{h_1}^\dagger a_{h_2}^\dagger}{\sqrt{1 - n_{h_1} - n_{h_2}}}.\end{aligned}\quad (43)$$

The eigenvalues correspond to those where one adds or removes two particles from the original ground state $|0\rangle$ with N particles. We again have to assume that the ground state is the vacuum to the addition operators, i.e. $A_p = 0$. Also the X^ρ , Y^ρ amplitudes have the orthonormality and completeness relations of standard p-RPA. We can define the removal operators

$$R_\alpha^\dagger = \frac{1}{2} \sum_{h_1 h_2} X_{h_1 h_2}^\alpha a_{h_2} a_{h_1} - \frac{1}{2} \sum_{p_1 p_2} Y_{p_1 p_2}^\alpha a_{p_2} a_{p_1}.\quad (44)$$

Again amplitudes can be determined from minimising a corresponding sum rule. The resulting RPA equations have a similar structure with (41) and (42). Actually the content of RPA equations for removal is the same as the one for addition. Only the amplitudes X^α , Y^α and X^ρ , Y^ρ have subtle relations involving interchange of $p \leftrightarrow h$ indices and relative phases.