RPA Selfconsistency and the killing condition

- 1) The Selfconsistent RPA
- 2) The SU(2) Lipkin model
- 3) RPA vacuum
- 4) Extension to O(5) algebra
- 5) The Agassi model
- 6) RPA and PBCS vacua (Preliminary results)

Brief review of the SCRPA

Defining:

$$Q_{\alpha}^{+} = \sum_{i} X_{i}^{\alpha} A_{i}^{+} - Y_{i}^{\alpha} A_{i}, \quad Q_{\alpha}^{+} |RPA\rangle = |\alpha\rangle, \quad Q_{\alpha} |RPA\rangle = 0$$

Minimization of the excited state leads to SCRPA equations:

$$\langle RPA | [H, Q_{\alpha}^{+}] | RPA \rangle = 0$$
 Generalized Mean Field

$$\left\langle RPA \middle| \left[A_i \left[H, Q_{\alpha}^{+} \right] \right] \middle| RPA \right\rangle = \omega_{\alpha} \left\langle RPA \middle| \left[A_i, Q_{\alpha}^{+} \right] \middle| RPA \right\rangle$$
$$\left\langle RPA \middle| \left[A_i^{+} \left[H, Q_{\alpha}^{+} \right] \right] \middle| RPA \right\rangle = \omega_{\alpha} \left\langle RPA \middle| \left[A_i^{+}, Q_{\alpha}^{+} \right] \middle| RPA \right\rangle$$

SCRPA

SCRPA is based on the preservation of the correlated GS as defined by the killing condition.

Replacement of

$$RPA \rangle \Rightarrow |HF\rangle$$

Immediately leads to HF + RPA.

In NP we have struggled to find the true RPA vacuum and/or a controlled approximation for determining the required expectation values.

In p-h RPA, using inversion and the killing condition, the expectation values required to close the system of equations are:

$$\langle c_{h_1}^+ c_{h_2} \rangle, \langle c_{p_1}^+ c_{p_2} \rangle, \langle c_{h_1}^+ c_{h_2} c_{h_3}^+ c_{h_4} \rangle, \langle c_{p_1}^+ c_{p_2} c_{h_3}^+ c_{h_4} \rangle, \langle c_{p_1}^+ c_{p_2} c_{p_3}^+ c_{p_4} \rangle.$$



The Lipkin Hamiltonian

$$H = \varepsilon J_0 - \frac{\chi}{2(\Omega - 1)} \left(J_+^2 + J_-^2 \right)$$

Single particle energy

Creates 2 p-h

Destroys 2 p-h

Symmetries:

$$\begin{bmatrix} H, J^2 \end{bmatrix} = 0, \quad \begin{bmatrix} H, J_i \end{bmatrix} \neq 0, \quad \begin{bmatrix} H, e^{i\pi J_0} \end{bmatrix} = 0$$

Choosing the representation $K=\Omega$, the states are:

$$\left|l\right\rangle = \sqrt{\frac{\left(\Omega - l\right)!}{l!\Omega!}} \left(J_{+}\right)^{l} \left|FS\right\rangle, \quad J_{-}\left|FS\right\rangle = 0, \quad J_{0}\left|FS\right\rangle = -\frac{\Omega}{2}$$

Low energy spectrum for Ω =40



The Selfconsistent RPA

J. Dukelsky and P. Schuck, Nucl. Phys. A 512, 466 (1990). HF transformation

$$\begin{pmatrix} a_{hm}^{+} \\ a_{pm}^{+} \end{pmatrix} = \frac{1}{\sqrt{1+x^{2}}} \begin{pmatrix} 1 & x \\ -x & 1 \end{pmatrix} \begin{pmatrix} c_{hm}^{+} \\ c_{pm}^{+} \end{pmatrix}$$

$$J_{+} = \frac{1}{1+x^{2}} \Big[2xK_{0} - x^{2}K_{-} + K_{+} \Big], \quad J_{0} = \frac{1}{1+x^{2}} \Big[\Big(1 - x^{2} \Big) K_{0} - x \Big(K_{-} + K_{+} \Big) \Big]$$

Where:

$$K_{0} = \frac{1}{2} \sum_{m} \left(a_{pm}^{+} a_{pm}^{-} - a_{hm}^{+} a_{pm}^{-} \right), \quad K_{+} = \sum_{m} a_{pm}^{+} a_{hm}^{-}$$

Generalized HF

$$\left\langle \begin{bmatrix} H, K_{+} \end{bmatrix} \right\rangle = 0$$

$$\frac{2x \left\langle K_{0} \right\rangle}{1 + x^{2}} \left\{ \varepsilon \left(1 + x^{2} \right) + \frac{\chi}{\left(\Omega - 1 \right)} \left(1 - x^{2} \right) \left[\left(\lambda + \mu \right)^{2} + 2 \left\langle K_{0}^{2} \right\rangle / \left\langle K_{0} \right\rangle \right] \right\} = 0$$

Generalized RPA

$$\begin{pmatrix} A & B \\ -B & -A \end{pmatrix} \begin{pmatrix} \lambda \\ \mu \end{pmatrix} = \omega \begin{pmatrix} \lambda \\ \mu \end{pmatrix}$$

Where

$$A = \frac{\left\{\varepsilon\left(1-x^{4}\right)+\frac{\chi}{\left(\Omega-1\right)}\left[-6x^{2}\left(\lambda^{2}+\mu^{2}\right)-12x^{2}\left\langle K_{0}^{2}\right\rangle /\left\langle K_{0}\right\rangle+2\left(1+x^{4}\right)\lambda\mu\left\langle K_{0}\right\rangle\right]\right\}}{\left(1+x^{2}\right)^{2}}$$

$$B = \frac{\chi \left[-12x^{2}\lambda\mu + (1+x^{4})(\lambda^{2} + \mu^{2}) + 2(1+x^{4})\langle K_{0}^{2} \rangle / \langle K_{0} \rangle \right]}{(\Omega - 1)(1+x^{2})^{2}}$$

The killing condition

The RPA operator is:

$$Q^{+} = \frac{1}{\sqrt{\Omega}} \left(\lambda K_{+} - \mu K_{-} \right), \quad \lambda^{2} - \mu^{2} = 1$$

Taking into account parity, the most general ansatz for the vacuum is:

$$\left|RPA\right\rangle = \sum_{l=0}^{\Omega/2} \alpha_{l} z^{l} \left(K_{+}\right)^{2l} \left|HF\right\rangle, \quad K_{-} \left|HF\right\rangle = 0, \ z = \frac{\mu}{\lambda}$$

Killing condition:

$$Q|RPA\rangle = 0 \Longrightarrow \alpha_l = \frac{(\Omega - 2l)!}{l!(\Omega/2 - l)!}$$

The expectation values needed to close the SCRPA equations are

$$\langle RPA | K_0 | RPA \rangle, \langle RPA | K_0^2 | RPA \rangle.$$

They can easily be calculated with the RPA vacuum, but let us explore possible approximations having in mind more general cases.

$$\left\langle K_{0}^{2}\right\rangle = \left\langle K_{0}\right\rangle^{2} + \frac{\left|\left\langle K_{0}Q^{+}Q^{+}\right\rangle\right|^{2}}{\left\langle QQQ^{+}Q^{+}\right\rangle} + O\left(Q^{4}\right) = \left\langle K_{0}\right\rangle^{2} + \frac{4\lambda\mu\left\langle K_{0}\right\rangle^{2}}{2\left\langle K_{0}^{2}\right\rangle + \left(\lambda^{2} + \mu^{2}\right)\left\langle K_{0}\right\rangle}$$

The other relation can be obtained from the SU(2) Casimir, or in the general case relating the two-particle density with the one-particle density

Is PBCS the vacuum of the p-h RPA in the Lipkin model?

Y. Ohrn and J. Linderberg, Int. J. Quantum Chem. 15, 343 (1979).

The answer is YES, but we have to extend the SU(2) algebra to incorporate pair operators.

The minimal extension is to the O(5) algebra, by adding the pair operators:

$$A_{p}^{+} = \sum_{m>0} c_{pm}^{+} c_{p-m}^{+}, A_{h}^{+} = \sum_{m>0} c_{hm}^{+} c_{h-m}^{+}, A_{0}^{+} = \sum_{m} \sigma_{m} c_{hm}^{+} c_{p-m}^{+}$$

PBCS is a pair condensate.

$$PBCS \rangle = \frac{1}{\left(\Omega/2\right)!} \left(A_{h}^{+} + zA_{p}^{+}\right) \left|0\right\rangle = \sum_{l=0}^{\infty} \frac{z^{l}}{\left(l!\right)^{2}} A_{p}^{+l}A_{h}^{l} \left|FS\right\rangle$$

It satisfies the Killing condition for Lipkin as well as in the general case. As demonstrated by Ohrn and Linderberg.

Does PBCS reflect the physics of the Lipkin model?

Ω=20



RPA ground state correlation energy for the different vacua



Comparison between exact and RPA excited states



The O(5) Agassi model

D. Agassi, Nucl. Phys. A 116, 49 (1968)

Figure 3. Phase diagram for the Agassi model when $N = \Omega$. Transition line A is given by $\chi = (\Omega - 1)(1 - \Sigma)$ and transition line B by $\chi = [(\Omega - 1)/(\Omega - 2)]\Sigma$.

Σ

The p-p RPA

Studies states of the system with $(\Omega+2)$ particles (additional phonon) and $(\Omega-2)$ particles (removal phonon), and the correlations induced in the system with Ω particles.

$$P^{+} = \frac{1}{\sqrt{\Omega}} \left(xA_{p}^{+} - yA_{h}^{+} \right), \quad R^{+} = \frac{1}{\sqrt{\Omega}} \left(yA_{p} - xA_{h} \right)$$

The killing condition defines a p-p RPA vacuum:

$$\left|RPApp\right\rangle = \sum_{l} z^{l} \left(A_{p}^{+}\right)^{l} \left(A_{h}^{+}\right)^{\Omega/2-l} \left|0\right\rangle$$

Comparison between three RPA vacuums

$$|RPAph\rangle = \sum_{l} \frac{\left(\Omega - 2l\right)!}{l!\left(\Omega / 2 - l\right)!} z^{l} \left(J_{+}\right)^{2l} |FS\rangle$$
$$|RPApp\rangle = \sum_{l} \frac{\left(\Omega / 2 - l\right)!}{l!} z^{l} \left(A_{p}^{+}\right)^{l} \left(A_{h}\right)^{l} |FS\rangle$$
$$|PBCS\rangle = \sum_{l} \frac{1}{\left(l!\right)^{2}} z^{l} \left(A_{p}^{+}\right)^{l} \left(A_{h}\right)^{l} |FS\rangle$$

Variational calculations for the three ansatz along the line $\chi=0$



normal to superconducting phase transition $\mathbf{0}$ -----*baa*a De la -2 Ø Exact 0 б<mark>8</mark>-4⊦ Ш PBCS **RPApp** -6 -8∟ -3 -2 2 0 3 -1 1 Σ

Some open questions

Could PBCS be the true p-h RPA vacuum in some region of the parameter space?

Is the formalism of p-h SCRPA equivalent to PBCS for systems with pairing correlations or even for superconductors?

In any case the study of RPA vacua deserve more attention.

The Agassi model seems to be a good benchmark model to understand and verify some of these questions.