Symmetry conserving coupled cluster doubles wave function and the self-consistent odd particle number RPA

M. Jemaï1,2,a, P. Schuck3,4,b

1 Laboratory of Advanced Materials and Quantum Phenomena, Physics Department, FST, El-Manar University, 2092 Tunis, Tunisia
2 ISSATM, Carthage University, Avenue de la République, P.O. Box 77, 1054 Amilcar, Tunis, Tunisia
3 Université Paris-Saclay, CNRS-IN2P3, IJCLab, 91405 Orsay Cedex, France
4 Université Grenoble Alpes, CNRS, LPMMC, 38000 Grenoble, France

Received: 4 August 2020 / Accepted: 7 October 2020 / Published online: 21 October 2020
© Società Italiana di Fisica and Springer-Verlag GmbH Germany, part of Springer Nature 2020
Communicated by Vittorio Somà

Abstract Mixing single and triple fermions an exact annihilation operator of the Coupled Cluster Doubles wave function with good symmetry was found in Tohyama and Schuck (Phys Rev C 87:044316, 2013). Using these operators with the equation of motion method the so-called self-consistent odd particle number random phase approximation (odd-RPA) was set up. Together with the stationarity condition of the two body density matrix it is shown that the annihilation conditions allow to reduce the order of correlation functions contained in the matrix elements of the odd-RPA equations to a fully self consistent equation for the single particle occupation numbers. Excellent results for the latter and the ground state energies are obtained in an exactly solvable model from weak to strong couplings.

1 Introduction

It is well known that the coupled cluster (CC) wave function is a powerful many-body ansatz. In this work we will use an approximation thereof, the so-called coupled cluster doubles (CCD) wave function. It is not easy nor straightforward to perform calculations with the CCD wave function. The technique most in use [2–4] is to project the equations for the ground state energy onto successively more complicated mp-mh configurations with m = 1, 2, ... and p, h single particle (s.p.) states above and below the Fermi level, respectively. Often excellent results have been obtained with these methods in various fields of physics (nuclear physics, chemistry, condensed matter, etc.) [3,4]. However, the method runs into difficulties when the system under consideration undergoes a transition to a spontaneously broken symmetry. A typical example is the transition to superconductivity of electronic systems or to super-fluidity of other Fermi systems like there are nuclear systems or cold atoms in traps. This is particularly relevant for finite systems where considering a definite number of particles can become mandatory. Very recently there have, thus, been attempts to formulate symmetry projected CCD approaches: (i) using BCS quasi-particle basis with projection to good particle number [5] (ii) an effort has also been undertaken for parity projection in the Lipkin model [6] (iii) also spin-projected CC has been applied to small-sized molecules [7]. Evidently such techniques lead to quite complex equations and to the best of our knowledge particle number projected CCD has not been applied to any realistic system so far.

In this paper we will go a different route leading certainly also to a theory of quite some unavoidable complexity but which presents in our opinion rather interesting aspects. In the recent past it was shown in [1] that the CCD wave function is the vacuum to exact annihilation operators mixing single and triple numbers of fermion operators. Taking those operators within an equation of motion (EOM) approach leads to the so-called self-consistent odd particle number RPA (odd-RPA) approach [1]. The problem is how to evaluate the matrix elements which contain up to three-body correlation functions appearing in this odd-RPA in a consistent way, since those operators which consist in a non-linear transformation of fermions cannot be inverted as it is the case with quasi particle operators obtained, e.g., from a Bogoliubov transformation among fermions. However, as we will show in this paper, there exists a way around. One namely can use the annihilation condition which mixes, as mentioned, single and triple fermion operators to reduce the order of correlation functions [8]. In applying this method successively, we will achieve that the matrix elements in odd-RPA only con-
tain correlated s.p. occupation numbers. To achieve this, one also has to take advantage in a last step of the stationarity of the two-body density matrix. We demonstrate the very good performance of this approach in applying it to the Lipkin model. This model is exactly solvable and frequently used to test many body techniques mostly in nuclear physics where it was invented but not only [9–18]. This model contains for test many body techniques mostly in nuclear physics.

To avoid confusion, let us say a word about the fact that CC theory contains already \( ph \) and \( pp \) RPA correlations [19]. Those correlations are of the standard RPA type. Not only the odd-RPA is quite different from standard \( ph \) and \( pp \) RPA in mixing single with triple fermion operators (standard RPA mixes doubles with doubles) but in addition a self-consistent scheme is set up. This self-consistency reduces under a certain approximation to symmetry broken Hartree–Fock (HF) equations, as will be discussed in the main text below. So the self-consistency in odd-RPA reflects the self-consistency contained in the HF equations, however, it is a selfconsistency which conserves good symmetry. Odd-RPA is, therefore, very different from RPAs contained in CC theory.

The paper is organised as follows. In Sect. 2 we present the general theory and in Sect. 3 we apply it to the Lipkin model. In Sect. IV, we outline and discuss our results, and in Sect. 5 we give our conclusions and present some perspectives. Finally in Appendix we give some detailed formulas.

### 2 General theory

In this paper we will consider the following CCD wave function

\[
|Z\rangle = \exp \left( \hat{Z} \right) |\text{HF}\rangle
\]

with

\[
\hat{Z} = \frac{1}{4} \sum_{pp'h'h'} z_{pp'h'h'} K_{ph}^{\dagger} K_{p'h'}^{\dagger}
\]

\[
= \frac{1}{4} \sum_{pp'h'h'} z_{pp'h'h'} P_{pp'}^{\dagger} P_{hh'}^{\dagger},
\]

where \( |\text{HF}\rangle \) is the Hartree–Fock (HF) Slater determinant and

\[
K_{ph}^{\dagger} = \beta_{p}^{\dagger} \beta_{h}^{\dagger} \quad K_{hp} = \beta_{h} \beta_{p}
\]

with \( \beta_{h}|\text{HF}\rangle = a_{h}^{\dagger}|\text{HF}\rangle = 0 \) and \( \beta_{p}|\text{HF}\rangle = a_{p}|\text{HF}\rangle = 0 \) (\( a_{k}^{\dagger}, a_{k} \) the fermion operators in the HF basis). The indices “\( p, p', \ldots \)” refer, as before, to single particle states ‘above’ and “\( h, h', \ldots \)” refer to single hole states ‘below’ the Fermi surface, respectively. The pair operators are given by

\[
P_{pp'}^{\dagger} = \beta_{p}^{\dagger} \beta_{p'}^{\dagger} \quad P_{hh'}^{\dagger} = \beta_{h}^{\dagger} \beta_{h'}^{\dagger}
\]

The amplitudes \( z_{pp'h'h'} \) must full-fill certain conditions so that the CCD state becomes the vacuum of the annihilation operators of this state (1). In addition, these amplitudes are anti-symmetric, i.e. if we change two indices of particles (or holes) we will have \( z_{pp'h'h'} = -z_{p'p'h'h} = z_{p'p'hh'h} \).

For an odd particle excitation operator, the annihilators can be defined as removal (\( \rho \)) mode or addition (\( \alpha \)) mode, respectively

\[
q_{\rho} = \sum_{h} x_{h}^{\rho} \rho_{h} + \sum_{pp'h'} U_{pp'h'}^{\rho} \rho_{p}^{\dagger} K_{p'h'}^{\dagger},
\]

\[
q_{\alpha} = \sum_{p} x_{p}^{\alpha} \alpha_{p} + \sum_{p'h'h'} U_{p'h'h'}^{\alpha} \alpha_{p}^{\dagger} K_{p'h'}^{\dagger},
\]

The annihilation conditions

\[
q_{\rho}|Z\rangle = 0,
\]

\[
q_{\alpha}|Z\rangle = 0,
\]

do not give the relations for the amplitudes as

\[
\sum_{h'} z_{pp'h'h'} x_{h'}^{\rho} = U_{pp'h'}^{\rho},
\]

\[
\sum_{p'} x_{p'}^{\alpha} z_{p'p'h'h'} = U_{p'h'h'}^{\alpha},
\]

For the case of pairing one must consider somewhat different annihilators, see\(^1\). In this paper we will, however, not consider the pairing case any further. It will be treated separately in a forthcoming paper. The coefficients \( x_{\rho}^{\rho} \); \( U_{\rho}^{\rho} \) will be determined from the extrema of sum rules for the average single particle energy,

\[
\lambda_{\rho} = \frac{\langle \{ q_{\rho}, [H, q_{\rho}^{\dagger}] \rangle \rangle}{\langle \{ q_{\rho}, q_{\rho} \} \rangle} \quad \text{or} \quad \lambda_{\alpha} = \frac{\langle \{ q_{\alpha}, [H, q_{\alpha}^{\dagger}] \rangle \rangle}{\langle \{ q_{\alpha}, q_{\alpha} \} \rangle}.
\]

\(^1\) The annihilators in the case of pairing are given by

\[
q_{\rho} = \sum_{h} y_{h}^{\rho} \rho_{h} + \sum_{pp'h'} V_{pp'h'}^{\rho} \rho_{p}^{\dagger} \rho_{h'}^{\dagger},
\]

\[
q_{\alpha} = \sum_{p} x_{p}^{\alpha} \alpha_{p} + \sum_{p'h'h'} V_{p'h'h'}^{\alpha} \alpha_{p}^{\dagger} \rho_{h'}^{\dagger},
\]

The annihilation conditions give the relations

\[
\sum_{h'} z_{pp'h'h'} y_{h'}^{\rho} = V_{pp'h'}^{\rho},
\]

\[
\sum_{p'} x_{p'}^{\alpha} z_{p'p'h'h'} = V_{p'h'h'}^{\alpha}.
\]
where [...] is the commutator, [...] is the anti-commutator and [...] = (Z...Z...), will be used throughout the paper. From the extrema of expressions (8), we obtain two coupled equations that written as a matrix eigenvalue equation have the following form

\[
\begin{pmatrix}
  e & C \\
  C^\dagger & D
\end{pmatrix}
\begin{pmatrix}
  x \\
  C
\end{pmatrix}
= \lambda
\begin{pmatrix}
  x \\
  C
\end{pmatrix},
\]  

(9)

with

\[
e_{hh'} = \langle\langle \beta_h [H, \beta_h^\dagger]\rangle\rangle,
\]

\[
C^a_{pp'h'h'} = \frac{\langle\langle [K_{hp'}^p, [H, \beta_{p'h'}^\dagger]]\rangle\rangle}{\sqrt{N_{pp'h'h'}}},
\]

\[
D_{pp'h', p1p2h'} = \frac{\langle\langle [K_{hp'}^p, [H, \beta_{p'h'}^\dagger]]\rangle\rangle}{\sqrt{N_{pp'h'h'}} \sqrt{N_{p1p2h'h'}}},
\]

\[
N_{pp'h'} = \langle\langle [K_{hp'}^p, \beta_{p'h'}^\dagger] K_{p'h'}^\dagger\rangle\rangle.
\]  

(10)

The two-body Hamiltonian is given by

\[
H = \sum_{kl} t_{kl} c_k^\dagger c_l + \frac{1}{4} \sum_{klmn} \tilde{v}_{klmn} c_k^\dagger c_l^\dagger c_m c_m,
\]  

(11)

with \(t_{kl}\) representing the matrix of the kinetic energy. The anti-symmetrised matrix elements of the two-body force are given by \(\tilde{v}_{kl} = (|k\rangle v|l\rangle - |l\rangle v'|k\rangle).\) A general two-body Hamiltonian in the HF-quasi-particle basis is given by [20]

\[
H = E_{HF} + H^{11} + H^{20} + H^{40} + H^{31} + H^{22}.
\]  

(12)

The different terms in (12) are given in “Appendix A”. We now proceed to the reduction of the order of correlation functions contained in the matrix elements of (10). We start with the following relations

\[
\beta_k[Z] = e^{\hat{\beta}_k \hat{Z}} \beta[Z],
\]  

(13)

with \(\beta_k = e^{-\hat{\beta}_k} \beta_k e^{\hat{\beta}_k} \) and

\[
\hat{\beta}_p = \beta_p + [\beta_p, \hat{Z}] + \text{zero}
\]  

(14a)

\[
\hat{\beta}_h = \beta_h + [\beta_h, Z] + \text{zero}
\]  

(14b)

where ‘zero’ means that the expansion has no further terms. This then yields the following relations

\[
\beta_p[Z] = \sum_{pp'h'h'} z_{pp'h'h'} K_{p'h'}^\dagger \beta_{p'h'}[\hat{Z}],
\]  

(15a)

\[
\beta_h[Z] = \sum_{pp'h'} z_{pp'h'} K_{p'h'}^\dagger \beta_{p'h'}[Z],
\]  

(15b)

which are just variants of the annihilation conditions. Now multiplying these relations from the left with \(\beta_h(\beta_p)\) and using (7), we arrive at a reduction of higher powers in \(K^\dagger\) to lower powers

\[
\sum_{p'p1h1h'} U_{pp'}^\rho h z_{p1p2h1h'} K_{p1h}^\dagger K_{p2h'}^\dagger |Z\rangle
\]

\[
= \delta_{pp'h} K_{h1}^\dagger |Z\rangle - (U_{p1}^\rho h - U_{pp'h}^\rho) K_{ph}^\dagger |Z\rangle,
\]  

(16a)

\[
\sum_{p1p'h1h2} U_{ph1h}^\alpha z_{p1p'h2h2} K_{p1h}^\dagger K_{p'h2h2}^\dagger |Z\rangle
\]

\[
= -\delta_{hh'} x_{p}^\alpha K_{hp}^\dagger |Z\rangle - (U_{phh'}^\alpha - U_{pp'h}^\alpha) K_{ph}^\dagger |Z\rangle.
\]  

(16b)

Similarly, we can reduce the even powers of \(K^\dagger\)

\[
\sum_{pp'} U_{pp'}^\rho h K_{pp'}^\dagger |Z\rangle = x_{h'}^\rho S_{hh'}[Z],
\]  

(17a)

\[
\sum_{hh'} U_{phh'}^\alpha K_{hh'}^\dagger |Z\rangle = -x_{p}^\alpha S_{pp'}[Z],
\]  

(17b)

where \(S_{hh'}\) and \(S_{pp'}\) are a density matrix operators \(S_{ij}\) given in “Appendix A’. From the mean value in the ground state (1), we find

\[
\langle S_{hh'} \rangle = \langle \beta_h^\dagger \beta_h \rangle
\]

\[
= \sum_{p} \langle \langle \beta_h^\dagger \beta_p \rangle \langle \beta_p \beta_h^\dagger \rangle \rangle = x_{h}^\rho (x_{p}^\rho)^\ast,
\]  

(18a)

\[
\langle S_{pp'} \rangle = \langle \beta_p^\dagger \beta_{p'} \rangle
\]

\[
= \sum_{a} \langle \langle \beta_p^\dagger \beta_{p'} \rangle \langle \beta_{p'} \beta_{p}^\dagger \rangle \rangle = x_{p}^\rho (x_{p'}^\rho)^\ast,
\]  

(18b)

and in particular, the s.p. occupation numbers as

\[
n_h = \langle \beta_h^\dagger \beta_h \rangle = |x_{h}^\rho|^2,
\]  

(19a)

\[
n_p = \langle \beta_p^\dagger \beta_p \rangle = |x_{p}^\rho|^2.
\]  

(19b)

Equations (16a, 16b) allow us to reduce higher powers to lower powers of \(K^\dagger\). For example, we multiply the equations (16) by \(K^\dagger\) on the left, we obtain correlation functions with the product of four operators \(K^\dagger\) expressed as a function of two operators only. From Eqs. (17a, 17b) and (18a, 18b), we can express all mean values quadratic in \(K^\dagger\) in terms of the density matrices \(\langle S_{pp'} \rangle\), \(\langle S_{hh'} \rangle\). Since mean values of products as \(\langle S_{kk}, S_{ll} \rangle\) (where \(k, k'\) or \(l, l'\) are two particle or two hole indices) appear in the Hamiltonian of Eq. (A1), we need one further relation to close the system of equations. It very naturally is given by demanding that the time derivative of the two body correlation function be zero, see also [22],

\[
i \frac{\partial}{\partial t} \langle \psi (t) | K_{ph}, K_{p'h'}^\dagger | \psi (t) \rangle = \langle \psi (t) | [H, K_{ph}^\dagger K_{p'h'}^\dagger] | \psi (t) \rangle,
\]

\[
= 0
\]  

(20)

where \(\psi (t) = \exp(-i H t) | Z \rangle\). It is this stationary condition of the two-body density matrix which gives us a relation
between the $\langle S_{kk'}S_{ll'} \rangle$ and $\langle S_{nm'} \rangle$,

$$\left\{ H, K_{ph}^\dagger K_{p'h'}^\dagger \right\} = \left\{ H, K_{hp} K_{h'p'} \right\} = 0.$$ (21)

For the explicit form of this commutator, see “Appendix A”. In order to test our theory, we choose the Lipkin model for an application. We also want to mention that we do not use any expansion of the CCD wave function as it is done usually when the CC theory is applied.

3 Application to the Lipkin model

The single-particle space of the Lipkin model consists of two fermion levels, each of which has a N-fold degeneracy see [9,20]. The upper (lower) level has the energy of $\frac{eJ}{2}$ ($-\frac{eJ}{2}$). The Hamiltonian of the Lipkin model is given by

$$H = eJ_0 - \frac{V}{2} \left( J_+^2 + J_-^2 \right),$$ (22)

with $e$ the inter-shell spacing, $V$ is the coupling constant, and

$$J_0 = \frac{1}{2} \sum_{m=1}^{N} (e_{1m}^+ c_{1m} - e_{0m}^+ c_{0m}) ,$$

$$J_+ = \sum_{m=1}^{N} c_{1m}^+ c_{0m}, \quad J_- = (J_+)^\dagger$$ (23)

with $2J_0 = \tilde{n}_1 - \tilde{n}_0, \tilde{n}_i = \sum e_{1m}^+ c_{1m}$ and $N$ the number of particles equivalent to the degeneracies of the shells. These operators obey the SU(2) algebra with the commutations rules

$$[J_+, J_-] = 2J_0, \quad [J_0, J_\pm] = \pm J_\pm.$$ (24)

The Lipkin model has been derived in nuclear physics and is, as mentioned in the Introduction, exactly solvable and frequently used to test many body approaches. The model is non-trivial and has a spontaneously discrete (parity) broken symmetry phase. Besides in nuclear physics, it is also considered in other fields of physics, see [10–17].

To proceed to the odd-RPA approach, we assume as variational ground state the CCD wave function given by the following expression

$$|Z\rangle = e^{iJ_+ J_0} |H F\rangle = e^{\tilde{Z}} |H F\rangle.$$ (25)

The ground state (25) is the vacuum for the two annihilators of normalised removal and addition modes, respectively,

$$q_\rho = \frac{1}{N} \sum_m \left[ x_0^+ e_{0m}^+ + U_0^\rho c_{1m}^+ J_+ \sqrt{\tilde{n}_{11}} \right],$$

$$q_\alpha = \frac{1}{N} \sum_m \left[ x_0^+ e_{1m} + U_1^\alpha c_{0m} J_- \sqrt{\tilde{n}_{11}} \right],$$ (26)

with $\tilde{n}_{11} = \langle c_{1m}^+ J_+, J_- c_{1m} \rangle = \langle c_{0m}^+ J_-, J_+ c_{0m} \rangle$. So we can verify the normalisation condition as

$$\langle q_\rho, q_\rho \rangle = |x_0^+|^2 + |U_0^\rho|^2 = 1$$

$$\langle q_\alpha, q_\alpha \rangle = |x_0^+|^2 + |U_1^\alpha|^2 = 1$$ (27)

Let us calculate the transformed single particle operators

$$\tilde{c}_{0m} = c_{0m} - z c_{1m} J_+, \tilde{c}_{1m} = c_{1m} + z J_+ c_{0m},$$ (28)

and consider the normalised amplitudes

$$\tilde{U}_0^\rho = \frac{U_0^\rho}{\sqrt{\tilde{n}_{11}}}, \quad \tilde{U}_1^\alpha = \frac{U_1^\alpha}{\sqrt{\tilde{n}_{11}}}.$$ (29)

Then the condition $q_\rho |Z\rangle = 0$ and $q_\alpha |Z\rangle = 0$ yields

$$z = \frac{\tilde{U}_0^\rho}{x_0^+} = \frac{x_0^+}{\sqrt{\tilde{n}_{11}}} = \frac{x_0^+}{\sqrt{\tilde{n}_{11}}} = -\frac{U_1^\alpha}{x_0^+ \sqrt{\tilde{n}_{11}}}.$$ (30)

We can find an expression of $J_0 |Z\rangle$ via $c_{0m} q_\rho |Z\rangle = 0$,

$$J_0 |Z\rangle = (\frac{N}{2} z + z J_+ J_0) |Z\rangle,$$ (31)

and for $J_- |Z\rangle$ via $c_{1m} q_\alpha |Z\rangle = 0$,

$$J_- |Z\rangle = z (\frac{N}{2} - J_0) J_+ |Z\rangle.$$ (32)

We can use the two equations (31) and (32) to find an expression for the correlation functions in terms of $\langle J_0 \rangle$ and $\langle J_0^2 \rangle$ (see more details in “Appendix B”).

It remains to express $\langle J_0^2 \rangle$ as a function of $\langle J_0 \rangle$. For this, one uses the stationary condition of the two bodies density (21),

$$0 = \langle [H, J_0^2] \rangle = 2e \langle J_0^2 \rangle - V \langle (2J_0 + 4J_0^2 - 4J_+ J_- J_0) \rangle.$$ (33)

Then, we obtain the following expression for $\langle J_0^2 \rangle$,

$$\langle 4J_0^2 \rangle = 2(2N - 3) \langle J_0 \rangle + 2 \frac{2V - ez}{V^2} \langle J_0^2 \rangle$$

$$-2(N-2) \langle J_+ J_- \rangle$$

$$= 2(2N - 3) \langle J_0 \rangle + 2 \frac{2V - ez}{V^2} \langle J_0 \rangle$$

$$-2(N-2) \langle J_+ J_- \rangle,$$ (34)

with $\langle J_+ J_- \rangle$ given in “Appendix B”. Finally all correlation functions are well expressed as a function of $z$ and $\langle J_0 \rangle$. Let us calculate the $\langle J_0 \rangle$ using the odd-RPA equations. We consider the conjugate of the annihilator of the ground state $|Z\rangle$ as odd excitation operator and we extremalize the energy (8) corresponding to these operators (26). We obtain a matrix eigenvalue equation for the two modes with the Hamiltonian matrix

$$h_{ij} = \begin{pmatrix} h_{00} & h_{01} \\ h_{10} & h_{11} \end{pmatrix}$$ (35)
and the corresponding secular equation
\[
\det(h - \lambda I) = 0. \tag{36}
\]

The normalisation factor \(\tilde{n}_{11}\) is given by
\[
\tilde{n}_{11} = \frac{1}{N} \sum_m \langle \{c_{1m}^\dagger J_+ , J_- c_{1m}\} \rangle
\]
\[
= \frac{1}{N} \sum_m \langle \{J_+ c_{0m} , c_{0m}^\dagger J_-\} \rangle
\]
\[
= (1 - \frac{2}{N}) \langle (J_+ J_-) - (J_0) \rangle + \frac{2}{N} \langle J_0^2 \rangle. \tag{37}
\]

For the first Hamiltonian element, we have
\[
h^\rho_{00} = \frac{1}{N} \sum_m \langle \{c_{0m}^\dagger , [H, c_{0m}]\} \rangle = \frac{e}{2}
\]
\[
h^\alpha_{00} = \frac{1}{N} \sum_m \langle \{c_{1m}^\dagger , [H, c_{1m}]\} \rangle = h^\rho_{00}
\]
and for the off diagonal elements
\[
h^\rho_{10} = h^\rho_{01} = \frac{1}{N \tilde{n}_{11}} \sum_m \langle \{c_{1m}^\dagger J_+ , [H, c_{0m}]\} \rangle = V \sqrt{\tilde{n}_{11}}
\]
\[
h^\alpha_{10} = h^\alpha_{01} = \frac{1}{N \tilde{n}_{11}} \sum_m \langle \{J_+ c_{0m} , [H, c_{1m}^\dagger]\} \rangle = h^\rho_{10}. \tag{39}
\]

The anti-commutator for \(h_{11}\) is given by
\[
h^\rho_{11} = \sum_m \langle \{c_{1m}^\dagger J_+, [H, J_- c_{1m}]\} \rangle
\]
\[
= - \frac{3e}{2} - \frac{2V}{N \tilde{n}_{11}} (N - 4) \langle (J_0^2) + (J_0^* J_0) \rangle
\]
\[
h^\alpha_{11} = \sum_m \langle \{J_+ c_{0m} , [H, c_{1m}^\dagger J_-]\} \rangle = h^\rho_{11}. \tag{40}
\]

Then Eq. (36) yields
\[
\lambda_\pm = - \frac{1}{2} (e - h_v) \pm \frac{1}{2} \sqrt{(2e + h_v)^2 + 4V^2 n_{11}} \tag{41}
\]
where \(h_v = \frac{2V}{N \pi_{11}} (N - 4) \langle (J_0^2) + (J_0^* J_0) \rangle\). So we can calculate
\[
n_0 = \sum_m |\langle c_{0m}^\dagger \lambda_+ \rangle|^2 = \sum_m |\langle (c_{0m}^\dagger , q_0, \rho) |_{E=\lambda_+} |^2 \tag{42}
\]
with \([c_{0m}^\dagger , q_\rho] = \lambda_+^\rho\). Then, the occupation numbers are given by
\[
n_0 = N |\lambda_+^\rho|^2 = N \frac{\lambda_+ - h_{11}}{\lambda_+ + \lambda_-} = N \frac{1}{1 + \lambda_- n_{11}} \tag{43}
\]

Thus (with \(n_1 = N - n_0\), we find
\[
\langle J_0 \rangle = \frac{N}{2} - n_0 = \frac{N}{2} \frac{\tilde{n}_{11}^2 - 1}{\tilde{n}_{11}^2 + 1}. \tag{44}
\]

With these relations the odd-RPA equation boils down to a non-linear relation for \(z\) which can easily be solved.

## 4 Results and discussion

Our main results are presented in Fig. 1. In the upper left panel, we show the expectation value of \(J_0\) which is related to the difference between the single particle occupation of the lower and upper levels as a function of the coupling constant \(\chi = V (N - 1)/e\) for particle number \(N = 8\). The exact result is given by the full line (black). The result of the present theory, i.e., odd-RPA, is given by the dotted line (red). The result where the CCD wavefunction is determined from the minimisation of the energy is represented by the full line with dots (purple). Finally the result from projected HF is shown by the broken line (blue). The result of standard RPA theory is displayed with the broken double-dot line (magenta). Needless to say that the standard RPA is very strongly improved by all the other three approaches. What is a particularly nice quality of the present approach (odd-RPA), is that it gives a very good approximation throughout the whole domain of couplings. Not surprisingly the same is true for the CCD wavefunction approach (min\([E_0(z)]\)) and for projected HF (min\([E_0^{CCD}(\delta)]\)).

In the upper right panel the same is repeated but for \(N = 40\). So we can calculate the exact result is still improved. The lower left panel shows the percentage error \(r = 100 \times (E_0^{odd-RPA} - E_0^{Exact})/E_0^{Exact}\). Here we see that odd-RPA and CCD approaches are very close while projected HF is a little worse. The lower right panel shows \(\langle J_0 \rangle\) which is related to the fluctuation of the occupation numbers as a function of \(\chi\). We remark a similar behaviour as for \(\langle J_0 \rangle\) in the upper left panel.

It is quite rewarding that odd-RPA represents a theory which (in the Lipkin model) yields results which go with good accuracy in a continuous way from weak to strong coupling passing smoothly through the (mean-field) phase transition point.

In Fig. 2, the two chemical potentials corresponding to the \(N \pm 1\) systems obtained with odd-RPA are compared with the exact values. Again very satisfying agreement is seen.

## 5 Conclusions and perspectives

It was known for a certain time that the CCD wave function is annihilated by well chosen combinations of single and triple fermion operators [1]. However, because of the non-linear fermion transformation, it remained an open problem how to deal with these operators. In this paper we showed that there exists a very efficient way how to manage a calculus with such operators. We showed that the more-body correlation functions appearing in the theory can be reduced to expectation values of the density operator with the help of the annihilation conditions and the stationarity of the two-body correlation function. The system of (odd-RPA) equations is then fully closed and calculations for s.p. occupation
Fig. 1  Upper left panel: the occupation number difference between upper and lower levels, $\langle -2J_0 \rangle$, for $N = 8$ with standard RPA (sRPA) (double dot broken line), present odd-RPA (dotted line), projected HF $\min\{E_0(\delta)\}$ (broken line), CCD variational wave function $\min\{E_0(z)\}$ (continuous line with dots), and exact solution (full line) as function of the intensity of interaction $\chi = \frac{V_e}{\tau}(N - 1)$. Upper right panel: $\langle -2J_0 \rangle$, for $N = 40$ with sRPA, odd-RPA, and exact solution. Lower left panel: For $N = 8$, percentage error $r$ of the correlation energy as odd-RPA (dotted line), CCD variational wave function (continuous line with dots) and projected HF (broken line) as function of the intensity of interaction $\chi$. Lower right panel: occupation fluctuation $\langle 4J_0^2 \rangle$ for $N = 8$ with same ingredients as upper left panel.

Fig. 2  The eigenvalues $\lambda_+$ and $\lambda_-$ of the odd-RPA matrix compared to the exact values as a function of $\chi$. 

N=8
numbers and ground state energies can be performed. We applied the theory to the Lipkin model with very good success. Indeed occupation numbers and correlation energies become excellent in the weak and remain very good in the strong coupling limits with numbers in between, that is in the transition region, which stay below 4% error. This is very satisfying. One may ask about the reason of this success. To this end, we remark that replacing in Eq. (5) the operators \( K_{ph}^\dagger \) by their expectation values, the non-linear transformation reduces to an ordinary linear HF-transformation among single fermion operators. The annihilation operators stand, therefore, for some sort of symmetry conserving quantum transformation of fermion operators. One may also say that the method consists of a symmetry conserving particle-vibration coupling (PVC) approach. In fact we performed calculations with parity projected HF wave functions (see (blue) broken lines in Fig.1) and also using the CCD wave function as a fully variational one (see (violet) lines with dots). We see that for the energies the latter two approaches are performing about the same as odd-RPA (with projected HF slightly worse) and also for the occupation numbers there is not a significant difference between all approaches.

In Sect. 2, we also briefly mentioned how to adapt odd-RPA to the pairing problem. This will be a task for the future. A still more ambitious project will be to apply our theory to the case of broken rotational symmetry. However, before, we shall gain more experience with this novel method for simpler cases. Another open problem to be considered in the future is the fact that there exist annihilators of the CCD wave function which contain an even number of fermion operators [21]. Those operators consist in a slight generalisation of the standard RPA \( ph \) operators. Similar procedures as we used here can certainly also be applied for those operators. It shall be very interesting to see how well excitation energies of collective nuclear states are reproduced.

Acknowledgements PS wants to thank Mitsuru Tohyama for past collaboration on odd-RPA. Discussions with Jorge Dukelsky are greatly acknowledged as well for suggestions and a careful reading of the manuscript.

Data Availability Statement This manuscript has no associated data or the data will not be deposited. [Authors’ comment: This is a theoretical study and no experimental data has been listed.]

Appendix A: Stationary condition

The stationary condition implies that the expectation value of the commutator \([ H, K_\uparrow K_\uparrow] \) must be zero with a general two-body Hamiltonian (12) where each elements are defined as,

\[
E_{HF} = \sum_h \epsilon_{hh} + \frac{1}{2} \sum_{hh'} \tilde{v}_{hh'h'h'},
\]

\[
H^{20} = \sum_{ph} (\epsilon_{ph} + \sum_{h'} \tilde{v}_{ph'h'h'}) K_{ph}^\dagger + \text{h.c.}
\]

\[
H^{40} = \frac{1}{4} \sum_{pp',hh'} \tilde{v}_{pp'h'h'} K_{ph}^\dagger K_{p'h'}^\dagger + \text{h.c.},
\]

\[
H^{11} = \sum_{pp} (\epsilon_{pp'} + \sum_{h} \tilde{v}_{php'h'}) S_{pp'} - \sum_{h'h} (\epsilon_{hh} + \sum_{h_1} \tilde{v}_{hh'h_1 h_1}) S_{hh'}
\]

\[
H^{31} = \frac{1}{2} \sum_{ph} K_{ph}^\dagger \left( \sum_{p'p_1} \tilde{v}_{pp'h_1 p_1} S_{p'p_1} + \sum_{h_1} \tilde{v}_{h_1 p_1 h', h_1} S_{h_1 h'} \right) + \text{h.c.},
\]

\[
H^{22} = \sum_{pp'h'} \tilde{v}_{ph'h'} K_{ph}^\dagger K_{p'h'}^\dagger + \frac{1}{4} \sum_{pp'} S_{pp'} + \frac{1}{4} \sum_{hh'} \tilde{v}_{hh'h_1 h_1} S_{hh'} - \frac{1}{4} \sum_{pp_1 p_2} \tilde{v}_{pp'p_1p_2} S_{pp_1} S_{p_1 p_2},
\]

where the density matrix operators \( S_{ij} \) are given by

\[
S_{hh'} = \beta_{h'h'}^\dagger \beta_{h'h'}, \quad S_{pp'} = \beta_{p'p'}^\dagger \beta_{p'p'}. \tag{A2}
\]

This Hamilton operator is exactly the same as the normal ordered one given in [20], Eqs (E.24) and (E.25). For later convenience we write it here in a slightly non normal ordered form. Let us then calculate this commutator with the general Hamiltonian (12),

\[
\left[ H^{11}, K_{ph}^\dagger K_{p'h'}^\dagger \right] = 2 \sum_{pp_1} \epsilon_{pp_1} K_{p'h_1}^\dagger K_{p'h'}^\dagger \tag{A3}
\]

\[
-2 \sum_{h_1} \epsilon_{hh_1} K_{ph_1}^\dagger K_{p'h'}^\dagger
\]

\[
\left[ H^{20}, K_{ph}^\dagger K_{p'h'}^\dagger \right] = \epsilon_{ph} K_{p'h'}^\dagger + \epsilon_{p'h'}^* K_{ph}^\dagger - \epsilon_{ph'}^* K_{p'h'}^\dagger \tag{A4}
\]

\[
-2 K_{ph}^\dagger \left( \sum_{h_1} \epsilon_{p'h_1} S_{h_1 h_1} + \sum_{p_1} \epsilon_{p_1 h_1} S_{p_1 p_1} \right)
\]

with

\[
\epsilon_{pp'} = t_{pp'} + \sum_{h_1} \tilde{v}_{ph_1 p_1 h_1},
\]

\[
\epsilon_{hh'} = t_{h'h'} + \sum_{h_1} \tilde{v}_{h_1 h_1 h_1},
\]

\[
\epsilon_{ph} = t_{ph} + \sum_{h_1} \tilde{v}_{ph_1 h_1}, \tag{A5}
\]
\[4\left[H^{40}, K^\dagger_{p'h'} K_{p'h'}\right] = -\sum_{p_1h_1} \bar{v}_{p_1h_1p'h'} K_{p'h'} K^\dagger_{p_1h_1} + \bar{v}_{p_1h_1p'h'} K^0_{p'h', h_1p_1} + \frac{1}{2} \sum_{p_1, p_2} \bar{v}_{p_1p_2pp_1} K^\dagger_{p_2h'} K_{p'h'} + \sum_{p_1, p_2h_1, h_2} \bar{v}_{p_1h_1h_2} K_{p'h_1} K^0_{p_2h_2} + \frac{1}{2} \sum_{h_2} \bar{v}_{h_1h_2h_1} K^\dagger_{h_2h_1} K_{p'h'}
\]

\[+2 \sum_{p_1, p_2h_1, h_2} \bar{v}_{p_1h_1h_2} K_{p_1h_1} K^0_{p_2h_2} + K^\dagger_{p'h'} K_{p'h_1} K^0_{h_1p_1} \]

\[+K^\dagger_{p'h'} K_{p'h_1} K^\dagger_{h_1p_1} \]

\[+\sum_{p_1h_1} \left( \bar{v}_{p_1h_1p'h'} + \bar{v}_{p_1h_1p'h_1} \right) K^\dagger_{p'h_1} K_{h_1p_1} \]

\[+\sum_{p_1h_1} \left( \bar{v}_{p_1h_1h_1} + \bar{v}_{p_1h_1h_1} \right) K^\dagger_{p'h_1} K_{h_1p_1} \]

\[-\sum_{p_1h_1} \left( \bar{v}_{p_1h_1p'h'} + \bar{v}_{p_1h_1p'h_1} \right) K^\dagger_{p'h_1} K_{h_1p_1} \]

\[-\sum_{h_1, h_2, h_3} \left( \bar{v}_{h_1h_2h_3} + \bar{v}_{h_1h_2h_3} \right) K_{p'h_1} K^0_{h_3h_2} \]

\[+\bar{v}_{h_1h_2h_3} K^\dagger_{p'h_1} K_{h_3h_2} \]

\[+\bar{v}_{h_1h_2h_3} K^\dagger_{p'h_1} + \bar{v}_{h_1h_2h_3} K^\dagger_{p'h_1} \]

\[\langle H, K^\dagger_{p'h'} K_{p'h'} \rangle = -\sum_{h_2} \bar{v}_{p_1h_1h_2} K^\dagger_{p'h_2} \]

\[+K^\dagger_{p'h'} \sum_{p_1h_1} K^\dagger_{p_1h_1} \left( \sum_{p_2} \bar{v}_{p_1p_2h_1p} K^\dagger_{p_2h_2} \right) - \sum_{h_2} \bar{v}_{p_1h_1h_2} K^\dagger_{p_1h_1} \]

\[+K^\dagger_{p'h'} \sum_{p_1h_1} \left( \sum_{p_2} \bar{v}_{p_1p_2h_1p} K^\dagger_{p_2h_2} \right) - \sum_{h_2} \bar{v}_{p_1h_1h_2} K^\dagger_{p_1h_1} \]

\[+K^\dagger_{p'h'} \sum_{p_1h_1} \left( \sum_{p_2} \bar{v}_{p_1p_2h_1p} K^\dagger_{p_2h_2} \right) - \sum_{h_2} \bar{v}_{p_1h_1h_2} K^\dagger_{p_1h_1} \]

\[+K^\dagger_{p'h'} \sum_{p_1h_1} \left( \sum_{p_2} \bar{v}_{p_1p_2h_1p} K^\dagger_{p_2h_2} \right) - \sum_{h_2} \bar{v}_{p_1h_1h_2} K^\dagger_{p_1h_1} \]

\[+K^\dagger_{p'h'} \sum_{p_1h_1} \left( \sum_{p_2} \bar{v}_{p_1p_2h_1p} K^\dagger_{p_2h_2} \right) - \sum_{h_2} \bar{v}_{p_1h_1h_2} K^\dagger_{p_1h_1} \]

\[\sum_{h_1, h_2, h_3} \left( \bar{v}_{h_1h_2h_3} + \bar{v}_{h_1h_2h_3} \right) K_{p'h_1} K^0_{h_3h_2} \]

\[+\bar{v}_{h_1h_2h_3} K^\dagger_{p'h_1} K_{h_3h_2} \]

\[+\bar{v}_{h_1h_2h_3} K^\dagger_{p'h_1} + \bar{v}_{h_1h_2h_3} K^\dagger_{p'h_1} \]

\[\langle H, K^\dagger_{p'h'} K_{p'h'} \rangle \]

\[= \delta_{p_1p_2} \delta_{h_1h_2} - \delta_{p_1p_2} S_{1h_2} - \delta_{h_1h_2} S_{p_1p_2} \]

\[\text{with} \]

\[K^0_{p_2h_2, h_1p_1} = \left[ K_{h_1p_1}, K^\dagger_{p_2h_2} \right] = \delta_{p_1p_2} \delta_{h_1h_2} - \delta_{p_1p_2} S_{1h_2} - \delta_{h_1h_2} S_{p_1p_2} \]

Summing the mean values of the different commutators in the ground state \( \langle Z \rangle \) for \( \langle H, K^\dagger_{p'h'} K_{p'h'} \rangle \) yields a relation between \( \langle S_{kk'}S_{ll'} \rangle \) and \( \langle S_{n'r'} \rangle \).

Appendix B: Calculation of correlation functions in the Lipkin model

All correlation functions can be expressed in terms of \( z, \langle J_0 \rangle \) and \( \langle J_0^2 \rangle \). We also have

\[n_0 = \frac{N}{2} - \langle J_0 \rangle, \quad n_1 = \frac{N}{2} + \langle J_0 \rangle \]

From the first Eq. (31), we find

\[z \langle J_1^2 \rangle = \frac{N}{2} + \langle J_0 \rangle \]

Multiplying (31) by \( J_1^2 \), gives

\[\langle J_1^2 J_0 \rangle = -\frac{N}{2} \langle J_1^2 \rangle + z \langle J_1^4 \rangle \]

which yields

\[2z \langle J_1^4 \rangle = N \langle J_1^2 \rangle + 2 \langle J_1^2 J_0 \rangle \]
Multiplying the second Eq. (32) by \( J_+ \), we can write
\[
\langle J_+ J_- \rangle = z(N - 1)\langle J_+^2 \rangle - z^2 \langle J_+^4 \rangle \tag{B5}
\]
which leads to
\[
z^2 \langle J_+^4 \rangle = (N - 1)z\langle J_+^2 \rangle - \langle J_+ J_- \rangle \tag{B6}
\]
Then, with (B4) and (B6), we find
\[
z\langle J_+^2 J_0 \rangle = \left( \frac{N}{2} - 1 \right)z\langle J_+^2 \rangle - \langle J_+ J_- \rangle \tag{B7}
\]
We multiply (31) from the left by \( J_0 \),
\[
J_0^2 |Z\rangle = -\frac{N}{2} J_0 |Z\rangle + z J_0 J_+^2 |Z\rangle = -\frac{N}{2} J_0 |Z\rangle + 2z J_+^2 |Z\rangle + z J_+^2 J_0 |Z\rangle \tag{B8}
\]
Replacing all terms of (B8) by their mean values, we find the Casimir relation
\[
\langle J_+ J_- |Z\rangle = \left( \frac{1}{4} N(N + 2) - J_0^2 + J_0 \right) |Z\rangle \tag{B9}
\]
In summary, the correlation functions are given by
\[
2z\langle J_+^2 \rangle = N + 2\langle J_0 \rangle
\]
\[
\langle J_+ J_- \rangle = \frac{1}{4} N(N + 2) - \langle J_0^2 \rangle + \langle J_0 \rangle
\]
\[
z\langle J_+^2 J_0 \rangle = \frac{1}{2} (N - 2)z\langle J_+^2 \rangle - \langle J_+ J_- \rangle
\]
\[
z\langle J_+ J_- J_0 \rangle = \frac{N}{2} (N + 2)z + \frac{1}{2} (N - 6)z\langle J_+ J_- \rangle - (N - 4)z\langle J_0 \rangle - \langle J_+^2 \rangle \tag{B10}
\]
what allows to solve the equation for \( \langle J_0 \rangle \).

References
1. M. Tohyama, P. Schuck, Phys. Rev. C 87, 044316 (2013)
2. J.P. Blaizot, G. Ripka, Quantum Theory of Finite Systems (MIT Press, Cambridge, 1986)
3. R.I. Bartlett, M. Musial, Rev. Mod. Phys. 79, 291 (2007)
4. G. Hagen, T. Papenbrock, M. Hjorth-Jensen, D.J. Dean, Rep. Prog. Phys. 77, 096302 (2014)
5. Y. Qiu, T.M. Henderson, T. Duguet, G.E. Scuseria, PRC 99, 044301 (2019)
6. J.M. Wahlen-Strothman, T.M. Henderson, M.R. Hermes, M. Degroote, Y. Qiu, J. Zhao, J. Dukelsky, G.E. Scuseria, J. Chem. Phys. 146, 054410 (2017)
7. Y. Qiu, T.M. Henderson, J. Zhao, G.E. Scuseria, J. Chem. Phys. 147, 064111 (2017)
8. I am very greatful to Virgil Baran who indicated this to me
9. H.J. Lipkin, N. Meshkov, A.J. Glick, Nucl. Phys. 62, 188 (1965)
10. S. Dusuel, J. Vidal, Phys. Rev. Lett. 93, 237204 (2004)
11. J. Vidal, G. Palacios, C. Aslangul, Phys. Rev. A 70, 062304 (2004)
12. P. Ribeiro, J. Vidal, R. Mosseri, Phys. Rev. Lett. 99, 050402 (2007)
13. G. Coló, S. De Leo, Int. J. Mod. Phys. E 27(5), 1850039 (2018)
14. O. Castanos, R. Lopez-Pena, J.G. Hirsch, Phys. Rev. B 74, 104118–14 (2008)
15. R. Puebla, A. Relano, Phys. Rev. E 92, 012101–9 (2015)
16. G. Coló, S. De Leo, Mod. Phys. Lett. A 30, 1550196–15 (2015)
17. S. Campbell, G. De Chiara, M. Paternostro, G.M. Palma, R. Fazio, Phys. Rev. Lett. 114, 177206–6 (2015)
18. J. Ripoche, T. Duguet, J.-P. Ebran, D. Lacroix, Phys. Rev. C 97, 064316 (2018)
19. Scuseria et al., J. Chem. Phys. 139, 104113 (2013)
20. P. Ring, P. Schuck, The Nuclear Many-Body Problem (Springer, Berlin, 1980)
21. M. Jemai, P. Schuck, Phys. Rev. C 100, 034311 (2019)
22. M. Tohyama, P. Schuck, Eur. Phys. J. A 19, 203 (2004)