Condensate Fragmentation in a New Exactly Solvable Model for Confined Bosons

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Based on Richardson’s exact solution of the multi level pairing model we derive a new class of exactly solvable models for finite boson system. As an example we solve a particular hamiltonian which displays a transition to a fragmented condensate for repulsive pairing interaction.

PACS number: 03.75.Fi, 05.30.Jp

Since the experimental realization of condensates of trapped bosonic atoms there exists a considerable growing interest in refining the approximations to study finite many body boson systems. Standard approaches used up to now are mean field based theories (MFT) like the Gross-Pitaevskii equation and the Bogoliubov theory which considers pair fluctuations on top of a Bose condensate. In order to test such many body approximations and also to gain insight, exactly solvable models are extremely useful. Two of such exactly solvable models were used in the context of boson traps, the one dimensional hard core boson model and the harmonic interaction model. Both model studies show the need to go beyond MFT. We would like to present in this letter a new class of exactly solvable models based on a generalization of Richardson’s exact solution of the pairing model. Of particular interest will be the model case with repulsive pairing interaction, where we find a fragmented condensate with two macroscopic eigenvalues of the one body density matrix corresponding to the lowest s and p wave states for bosons in a confining potential. The occurrence of condensate fragmentation in confined boson systems is a much debated subject at present and so far no clear evidence for the existence of such a state has been demonstrated. Nozières and Saint-James using the Hartree-Fock Bogoliubov (HFB) approximation and later on Nozières using Hartree-Fock (HF) theory showed that fragmentation is energetically unfavoured with respect to a single condensate state for scalar boson systems. Going beyond mean field Holzmann et.al. discussed the possible existence a fragmented scalar boson condensate in two dimensions. The case of trapped spin 1 boson systems has been treated in refs. where it was concluded that fragmentation might be realized in spin space but they still used mean field theory to describe the condensates in each spin component.

Let us now come to the construction of our new exactly solvable model for interacting bosons. In ref. Richardson was able to obtain the exact eigenstates of a pairing hamiltonian for bosons

$$H_P = \sum_\Lambda \varepsilon_\Lambda n_\Lambda + \frac{g}{2} \sum_{\Lambda \Lambda'} A_\Lambda A_{\Lambda'}$$

(1)

where $A_\Lambda = \sum_\alpha a_{\Lambda \alpha} a_{\Lambda \alpha}^\dagger$, $n_\Lambda = \sum_\alpha a_{\Lambda \alpha}^\dagger a_{\Lambda \alpha}$, $(\Lambda \alpha)$ are the quantum numbers of a confining potential (in the particular example of a three dimensional spherical potential which we will discuss below $\Lambda$ is the principal quantum number and $\alpha$ represents the orbital quantum numbers), and $(\Lambda \alpha)$ is the time reversal of $(\Lambda \alpha)$. The operator $A_\Lambda$ creates a zero angular momentum pair (singlet) in level $\Lambda$ and the operator $n_\Lambda$ counts the number of bosons in level $\Lambda$.

In analogy with the solution for fermions Richardson assumed that the hamiltonian eigenstates can be written as a pair product wave function of the form

$$|\psi\rangle = \prod_{i=1}^N B_i^\dagger |\varphi\rangle$$

(2)

where $B_i^\dagger = \sum_\Lambda \frac{1}{\varepsilon_\Lambda - E_i} A_\Lambda^\dagger$. $N$ is the number of singlet boson pairs, $E_i$ are pair energies to be determined by the eigenvalue equation and $|\varphi\rangle$ is a state of $\nu$ unpaired bosons that fulfills $A_\Lambda |\varphi\rangle = 0$ and $n_\Lambda |\varphi\rangle = \nu_{\Lambda} |\varphi\rangle$. A given configuration in the Hilbert space is determined by the set $\nu_{\Lambda}$ of unpaired bosons in each level $\Lambda$. The total number of bosons is then $N = 2N + \sum_{\Lambda} \nu_{\Lambda}$. A crucial point is the observation that the off diagonal matrix elements of the one body density matrix $\langle \psi | a_{\Lambda \alpha}^\dagger a_{\Lambda' \alpha'} | \psi \rangle$ are zero with $|\psi\rangle$ given by (2) because the action of $a_{\Lambda \alpha}^\dagger a_{\Lambda' \alpha'}$ on $|\psi\rangle$ either destroys a singlet pair increasing $\nu$ or 2 or it acts on an unpaired particle changing its configuration from $(\Lambda \alpha)$ to $(\Lambda' \alpha')$. In any case the state $a_{\Lambda \alpha}^\dagger a_{\Lambda' \alpha'} | \psi \rangle$ with $\Lambda \alpha \neq \Lambda' \alpha'$ will be orthogonal to $|\psi\rangle$. Therefore the occupation numbers $\langle \psi | n_{\Lambda} | \psi \rangle$ are the eigenvalues of the one body density matrix. This situation is analogous to the Fermion case where this is known as the generalised seniority scheme.

By acting with the hamiltonian on the trial wavefunction, after a straightforward but long derivation, Richardson obtained the following set of equation for the pair energies

$$1 + g \sum_{\Lambda} \frac{(\Omega_{\Lambda} + 2\nu_{\Lambda})}{(2\varepsilon_\Lambda - E_i)} + 4g \sum_{j \neq i} \frac{1}{E_j - E_i} = 0$$

(3)

where $\Omega_{\Lambda}$ is the degeneracy of level $\Lambda$. The energy eigenvalues of (3) are given by $E = \sum_{\Lambda} \varepsilon_\Lambda \nu_{\Lambda} + \sum_{i=1}^N E_i$ for each solution of the set of equations (3) as will be explained below.

The proof of integrability of the pairing model for fermion systems has been given by Cambiaggio et al.
The authors found a complete set of commuting operators (constants of motion) in terms of which it is possible to express the pairing hamiltonian and the number operators as particular linear combinations. Unfortunately, since the authors were not aware of the Richardson’s previous works, they were not able to obtain the eigenvalues of the new set of operators, nor the exact solution of the pairing hamiltonian. This connection has been established recently [13] and the eigenvalues of the commuting operators found using Conformal Field Theory.

The Richardson solution for fermions remained practically unused till very recently when it was applied, in the context of ultrasmall superconducting grains [16], to study the transition from the superconducting to the normal state. We are not aware of any application for boson systems.

In complete analogy to the fermion case, a set of global commuting operators can also be written in the boson case, based on the group algebra of the pseudo-spin generators $K_{A}^{0} = \frac{1}{2}u_{A} + \frac{1}{2}\Omega_{A}$, $K_{A}^{+} = \frac{1}{2}A_{A} = (K_{A}^{-})^{\dagger}$ of $SU(1, 1)$.

$$R_{\Lambda} = K_{\Lambda}^{0} + 2g \sum_{\Lambda' \neq \Lambda} \frac{1}{\eta_{\Lambda} - \eta_{\Lambda'}} K_{\Lambda} \cdot K_{\Lambda'}$$

(4)

The scalar product in (4) refers to the $SU(1, 1)$ group, $K_{\Lambda} \cdot K_{\Lambda'} = \frac{1}{2} (K_{\Lambda}^{+} K_{\Lambda'} + K_{\Lambda'}^{+} K_{\Lambda}) - K_{\Lambda}^{0} K_{\Lambda'}^{0}$. The set of operators $R_{\Lambda}$ is complete, the operators commute among each other, and the pairing hamiltonian (1) can be written as the linear combination $2 \sum_{\Lambda} \eta_{\Lambda} R_{\Lambda}$. These conditions demonstrate that the pairing model is integrable for boson systems.

We will now look for the eigenstates of the $R_{\Lambda}$ operators (4) using the trial eigenstates (3). The form of the boson pair amplitudes $u^{i}_{A}$ in the boson pair operators $B_{A} = \sum_{A} u^{i}_{A} A_{A}$ is fixed by the solution of the one pair problem, namely $u^{i}_{A} = 1/(2\eta_{A} - E_{i})$. The eigenvalues $R_{\Lambda} |\psi\rangle = \lambda_{\Lambda} |\psi\rangle$ can be worked out in an analogous way as in the original Richardson paper. The eigenvalues are given by

$$\lambda_{\Lambda} = \frac{\Sigma_{\Lambda}}{2} \left[ \frac{1}{2} - 2g \sum_{i} \frac{1}{2\eta_{\Lambda} - E_{i}} - \frac{g}{4} \sum_{\Lambda' \neq \Lambda} \frac{\Sigma_{\Lambda'}}{\eta_{\Lambda} - \eta_{\Lambda'}} \right]$$

(5)

where $\Sigma_{\Lambda} = \Omega_{\Lambda} + 2\eta_{\Lambda}$, while the pair energies $E_{i}$ should be the roots of the Richardson equations (3) with $\eta_{\Lambda}$ replacing $\varepsilon_{i}$.

One can readily verify that for $\eta_{\Lambda} = \varepsilon_{\Lambda}$ in eqs. (3) and (4), the linear combination $2 \sum_{\Lambda} \varepsilon_{\Lambda} R_{\Lambda}$ gives the Richardson hamiltonian (1) and $2 \sum_{\Lambda} \varepsilon_{\Lambda} \lambda_{\Lambda}$ gives the corresponding eigenvalue. An important by-product of having found the eigenvalues (4) is that the $\eta_{\Lambda}$ are in principle free parameters not necessarily related to the single boson energies. We will exploit this freedom to obtain solutions for generalized pairing hamiltonians.

Looking back to the form of the hamiltonian (1) one sees that since the pair operators $A_{\Lambda}$ are normalized to the square root of the degeneracy of the level $\Lambda$, the effective pairing matrix elements are proportional to the square root of the product of the degeneracies of the two shells $\sqrt{\Omega_{\Lambda}\Omega_{\Lambda}}$. In a spherical harmonic oscillator potential each degeneracy is in turn proportional to $\Lambda^{d-1}$ where $d$ is the space dimension and $\Lambda$ is the principal quantum number while the single boson energies are linear in $\Lambda$, producing unphysical occupations of the high lying levels for attractive pairing or a compression of the bosons in the lowest level for repulsive pairing. We will obtain a more realistic hamiltonian making use of the freedom in the choice of the $\eta_{\Lambda}$. In order to cancel the undesired dependence of the effective pairing matrix elements on the degeneracies we make the following definition $\eta_{\Lambda} = (\varepsilon_{\Lambda})^{d}$ in eqs. (4) and (5). The new hamiltonian $H = 2 \sum_{\Lambda} \varepsilon_{\Lambda} R_{\Lambda}$ can be expanded using the definition of the $R_{\Lambda}$ (4) in terms of the $SU(1, 1)$ generators or equivalently in terms of the pair operators. The final form of the hamiltonian is (more details of its construction will be given elsewhere)

$$H = \mathcal{E} + \sum_{\Lambda} \varepsilon_{\Lambda} n_{\Lambda} + \sum_{\Lambda\Lambda'} V_{\Lambda\Lambda'} \left( A_{\Lambda}^{\dagger} A_{\Lambda'} - n_{\Lambda} n_{\Lambda'} \right)$$

(6)

with $\mathcal{E}$ an uninteresting constant, $\varepsilon_{\Lambda} = \varepsilon_{\Lambda} + 2V_{\Lambda\Lambda} - \sum_{\Lambda'} V_{\Lambda\Lambda'} \Omega_{\Lambda'}$ being the single boson energies, and $V_{\Lambda\Lambda'} = g/2 \sum_{l=0}^{d-1} \frac{\varepsilon_{\Lambda}^{d-1-l}}{\Lambda^{d-1-l}}$.

We can readily check that now the effective interaction terms in (6), contrary to (1), correctly scale with energy. In addition to the pairing term in (6) also appears a particle-hole interaction of the monopole-monopole type which gives the hamiltonian a rather rich and quite general character. It has, however, the restriction that pairing and particle-hole interactions are linked to be of opposite sign, a feature which may be realised only in particular situations. On the other hand, we think that the equality in magnitude of both interactions does not invalidate our general conclusions below.

The energy eigenvalues of (6) can be obtained summing the eigenvalues (4) as

$$E = \frac{1}{2} \sum_{\Lambda} \varepsilon_{\Lambda} \Sigma_{\Lambda} - \frac{1}{4} \sum_{\Lambda \neq \Lambda'} \Sigma_{\Lambda} \Sigma_{\Lambda'} V_{\Lambda\Lambda'} - 2g \sum_{\Lambda} \frac{\varepsilon_{\Lambda} \Sigma_{\Lambda}}{2\eta_{\Lambda} - E_{i}}$$

(7)

It is worthwhile to emphasize at this point that the states (2) are common eigenstates of the operators $R$ in (6) and, consequently, of any linear combination of them like the pairing hamiltonian (1) or our more general hamiltonian (6) provided that the pair energies are the solutions of equation (3). The solution of (3) was already discussed in ref. [14] and we will give here only a
brief summary. Assuming that we have \( L \) oscillator levels and \( 2\mathcal{N} \) paired bosons, the \( \mathcal{N} \) pair energies \( E_i \) are real roots of \((3)\) in the interval \(-\infty < E_i < 2\eta_L\) for an attractive pairing interaction or \(2\eta_0 < E_i < \infty\) for a repulsive pairing interaction. The groundstate has all pair energies in the restricted intervals \(-\infty < E_i < 2\eta_0\) for an attractive pairing interaction or \(2\eta_0 < E_i < 2\eta_1\) for a repulsive pairing interaction. Any state in the Hilbert space corresponds to a particular distribution of the \( \mathcal{N} \) pair energies into the \( L \) intervals. States with broken pairs can be generated by replacing a boson pair \( \mathcal{B} \) by two unpaired bosons which can occupy any of the \( L \) shells. For example, the first excited state with two unpaired bosons corresponds to solve \((3)\) with \( \mathcal{N} - 1 \) pair energies in the first possible interval and \( \nu_0 = \nu_1 = 1 \).

Having in mind that the eigenstates of the hamiltonian \((1)\) are the same as those of the pairing hamiltonian \((1)\), the occupation numbers for a given state can be calculated as the derivatives of the pairing hamiltonian \( H_P \) \((1)\) with respect to the the single boson energies \( \varepsilon \) as has been done by Richardson in \[12\]

\[
\langle n_\Lambda \rangle = \left\langle \frac{\partial H_P}{\partial \varepsilon_\Lambda} \right\rangle = \nu_\Lambda + \sum \frac{\partial E_i}{\partial \varepsilon_\Lambda} \tag{8}\]

Details of the derivation of the occupation numbers and the final set of equations can be found in ref. \[12\].

![FIG. 1. Occupation numbers for 1000 bosons in 50 harmonic oscillator shells, the interaction strength is \( g = -2.0 \), giving a depletion factor of 0.608.](image)

We have performed a series of calculations for a system of 1000 bosons (\( \mathcal{N} = 500 \)) trapped in a three dimensional spherical harmonic oscillator with a cutoff at \( 101/2 \hbar \omega \) \((L = 50)\). For attractive pairing all quantities evolve smoothly with increasing attraction. In fig. 1 we show the occupation numbers for \( g = -2.0 \) corresponding to a depletion factor of 0.608. They display a reasonable pattern filling first the lowest levels. This is not the case for the pairing hamiltonian \((1)\) with \( \eta_\Lambda = \varepsilon_\Lambda \) which for \( d > 1 \) populates first the high lying levels. The comparison between the exact results and approximations like Hartree-Fock-Bogoliubov or their number conserving extensions \[7,8\] will be the topic of a future work \[19\].

Changing now to repulsive pairing we have found an unexpected feature. For some critical value of \( g \) the normal groundstate boson condensate suddenly turns into a state in which the bosons are condensed into the \( \Lambda = 0 \) and the \( \Lambda = 1 \) states while the occupation of the other levels is negligible. This state was already envisaged by Richardson himself studying an approximate solution for eq. \((3)\) in the thermodynamic limit \[12\]. Taking into account that the one body density matrix is diagonal in the basis \( (\alpha \Omega) \) (see above) the occupation numbers in \((8)\) are their diagonal matrix elements or, equivalently, the density matrix eigenvalues. Therefore, this new state with a macroscopic occupation of the two lowest harmonic oscillator shells constitutes a truly fragmented condensate state. It is commonly accepted since the work of Nozieres and Saint James \[8\] that for homogeneous systems fragmentation cannot occur in systems of scalar bosons with repulsive interactions. This might perhaps be the first example of fragmentation in a confined boson systems.

In order to understand the nature of this new quantum phase we consider a coherent state \( |\phi \rangle = \exp \left[ \sqrt{2\mathcal{N}} a_{111}^\dagger |0\rangle \right] \) where \( \Gamma \) is the most general time reversal invariant coherent boson that breaks rotational and reflection symmetry.

\[
\Gamma = \frac{1}{\sqrt{1 + \beta^2}} \left[ a_0^\dagger + \beta \cos \gamma \ a_{111}^\dagger \right]
\]

\[
\beta \sin \gamma \left( e^{i\varphi} a_{111}^\dagger - e^{-i\varphi} a_{111}^\dagger \right)
\]

where the three independent variables are defined in the intervals \( \beta \geq 0, \ 0 \leq \gamma \leq \pi \) and \( 0 \leq \varphi \leq 2\pi \).

Since, as mentioned before, the groundstate is a common eigenstate to our hamiltonian \((1)\) and to the pairing hamiltonian \((1)\) with \( \eta_\Lambda = (\hbar \omega \Lambda + 3/2)^3 \), for simplicity we minimize the energy of the latter hamiltonian which, indeed, will turn out to be a very accurate procedure. Apart from a constant energy term, the groundstate energy and the occupation numbers are given by

\[
E = \frac{\beta^2}{1 + \beta^2} + x \frac{(1 - \beta^2)^2}{4(1 + \beta^2)^2} \tag{10}\]

\[
\nu_0 = \frac{2\mathcal{N}}{1 + \beta^2}, \ \nu_1 = \frac{2\mathcal{N} \beta^2}{1 + \beta^2} \tag{11}\]
where we have defined the adimensional parameter $x = \frac{4N\bar{g}}{\hbar\omega}$. The energy $\langle 0 \rangle$ is independent of the variational parameters $\gamma$ and $\varphi$. Minimization of $\langle 0 \rangle$ with respect to $\beta$ gives the solutions $\beta = 0$ for $x \leq 1$ and $\beta = \sqrt{\frac{x - 1}{x + 1}}$ for $x > 1$. The critical interaction strength corresponding to the phase transition at $x = 1$ is $g_c = \frac{\pi}{2x}$. On the other hand, it is easy to check that the Bogoliubov approximation has a break down at this critical value of $g$ showing the instability of the singlet boson condensate against pair fluctuations. Beyond the critical point the occupation numbers for the first two levels, obtained by inserting the minimum $\beta$ value in $\langle 0 \rangle$, are $n_0 = \frac{x+1}{2x}$ and $n_1 = \frac{x-1}{2x}$.

![FIG. 2. Occupation numbers $n_0$ and $n_1$ for 1000 bosons in 50 harmonic oscillator shells as a function of the adimensional parameter $x$.](image)

In figure 2 we have plotted the occupation numbers of the first two levels for a system of 1000 bosons interacting in 50 levels of a three dimensional harmonic oscillator as a function of the parameter $x$. The exact results in solid lines clearly display an abrupt transition for $x = 1$ as predicted by the meanfield description. In fact the approximate results are indistinguishable from exact ones. Moreover the total occupation of the rest of the levels is always lower than $10^{-2}$. We have added two insets to the figure to show a close up of the transition region for the occupations $n_0$ and $n_1$. The small differences between the exact and the approximate results suggest that this is a $1/N$ effect, and that we are seeing the precursor of a true quantum phase transition.

The new phase is a rather peculiar fragmented state characterized by a macroscopic occupation of only the two lower levels. It can be approximated by a single condensate state at the price of breaking of the reflection symmetry generating a permanent dipole deformed state. As we have seen before the parameter $x$ is proportional to the number of bosons and inversely proportional to the oscillator frequency. Assuming that this phase transition might be realized in realistic systems, it can be controlled by varying the number of bosons or the characteristics of the confining potential.

In conclusion, we have developed a new class of exactly solvable models for confined boson systems. These models are exactly solvable in any dimension (reflected in the degeneracies $\Omega_\Lambda$) and with any kind of confining potential (reflected in the single boson energies $\varepsilon_\Lambda$). We have made numerical applications showing the great potential utility of the model for serving as a testing tool for many body approximations. Moreover we have found a quantum phase transition to a fragmented state for repulsive pairing interactions. To the best of our knowledge, this is the first example of fragmentation in a confined scalar boson system. As such, it may stimulate further investigations to see whether this new phase can arise in more realistic situations.

**Acknowledgments** We thank G. Sierra and G.G. Dussel for fruitful conversations. This work was supported in part by the DGES spanish grant PB98-0685.

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