Exactly solvable models for triatomic-molecular Bose-Einstein Condensates

G. Santos[1]**, A. Foerster**[2]**, I. Roditi**[1]**,**
Z. V. T. Santos[1] **and A. P. Tonel**[3]

[1]CBPF - Centro Brasileiro de Pesquisas Físicas, Rio de Janeiro, RJ - Brazil
[2]Instituto de Física da UFRGS, Porto Alegre, RS - Brazil
[3]CCET da Universidade Federal do Pampa/Unipampa, Bagé, RS - Brazil

E-mail: `gfilho@cbpf.br`

Abstract. We construct a family of triatomic models for heteronuclear and homonuclear molecular Bose-Einstein condensates. We show that these new generalized models are exactly solvable through the algebraic Bethe ansatz method and derive their corresponding Bethe ansatz equations and energies.

PACS numbers: 02.30.Ik, 03.65.Fd, 03.65.-w, 05.30.Jp, 03.75.Nt

1. Introduction

Since the pivotal experimental achievement that led to realizations of Bose-Einstein condensates (BECs), using ultracold dilute alkali gases [1, 2], a great effort has been devoted to the understanding of new properties of BEC. The creation of a molecular BEC compound, which has been obtained by different techniques [3], leads one also to the compelling chemistry of BECs, where the atomic constituents may form molecules, for instance, by Feshbach resonances [4] or photoassociation [5]. These results turned the search for integrable models that could be candidates for describing BEC properties into a very active field of research [6, 7, 8, 9, 10, 11, 12]. In fact, exactly solvable models are expected to provide a significant impact in this area, a view that has been promoted in [13, 14].

Moreover, the recent experimental evidence for Efimov states in an ultracold cesium gas [15] provided a physical ground for the search of tri-atomic homonuclear molecular BECs. Due to the rapid technological developments in the field of ultracold systems, this experiment is just the beginning of the study of tri-atomic molecules [16, 17].

We introduce, in the present paper, a complete family of new solvable models for both heteronuclear and homonuclear *tri-atomic* molecular BECs obtained through a combination of two Lax operators constructed using special realizations of the $su(2)$ and $su(1,1)$ algebras, as well as a multibosonic representation of $sl(2)$, discussed recently in [18].

Until now, integrability was shown for those Hamiltonians describing heteronuclear and homonuclear *di-atomic* molecular BECs [7]. In the heteronuclear case, two different atoms, labelled a and b, can be combined to produce a molecule labelled by c. The different degrees of freedom in such models are represented by canonical creation and annihilation operators $\{a, b, c, ..., a^\dagger, b^\dagger, c^\dagger, ...\}$ satisfying the usual commutation relations $[a, a^\dagger] = I$, etc., and commuting among different species. The Hamiltonian for the *di-atomic* heteronuclear model reads [7, 19]

$$
\begin{aligned}
H = {} & U_{aa}N_a^2 + U_{bb}N_b^2 + U_{cc}N_c^2 + U_{ab}N_aN_b + U_{ac}N_aN_c + U_{bc}N_bN_c \\
& + \mu_a N_a + \mu_b N_b + \mu_c N_c + \Omega(a^\dagger b^\dagger c + c^\dagger ba).
\end{aligned}
\tag{1}
$$

The parameters U_{ij} describe S-wave scattering, μ_i are external potentials and Ω is the amplitude for interconversion of atoms and molecules. In the homonuclear case, two identical atoms labelled a are combined to produce a molecule c [7]. The generalization to the triatomic case is not immediate and in particular, for the homonuclear case, a one mode multibosonic realization of $sl(2)$ is essential.

In what follows we will show that it is possible to find other integrable generalized molecular BEC models, more specifically, heteronuclear and homonuclear *tri-atomic* models. We first introduce two models, one with two identical species of atoms and a different one and another model where there are three different species of atoms. In both cases the three atoms can be combined to form a molecule. We then introduce a model consisting of three identical species of atoms which uses a recently defined multibosonic

realization of the $sl(2)$ algebra [18]. We present how these generalized models can be derived from a transfer matrix, thus allowing us to show their integrability by the algebraic Bethe ansatz method. We also obtain their corresponding energies and Bethe ansatz equations.

2. Triatomic molecular models

We are going to introduce in this section three different Hamiltonians describing triatomic-molecular BECs, two for the hetero-atomic case and one for the homo-atomic case. We are considering the coupling parameters real, such that the Hamiltonians are hermitian. The U parameters describe the S-wave scattering, the μ parameters are the externals potentials and Ω is the amplitude for interconversion of atoms and molecules. The operators N_j, $j = a$, b, c, d are the number operators acting in the Fock space.

2.1. Heteronuclear molecular models

We can construct two models for hetero-atomic molecular BECs, one with two identical species of atoms and a different one and another model where there are three different species of atoms.

2.1.1. Model for 2 atoms a and 1 atom b
The Hamiltonian that describes the interconversion of a heterogeneous tri-atomic molecule labelled by c with two atoms of type a and one atom of type b is given by

$$
\begin{aligned}
H = {} & U_{aa}N_a^2 + U_{bb}N_b^2 + U_{cc}N_c^2 + U_{ab}N_aN_b + U_{ac}N_aN_c + U_{bc}N_bN_c \\
& + \mu_a N_a + \mu_b N_b + \mu_c N_c + \Omega(a^\dagger a^\dagger b^\dagger c + c^\dagger baa).
\end{aligned}
\tag{2}
$$

This Hamiltonian (2) has two independent conserved quantities,

$$
\begin{aligned}
I_1 &= N_a + 2N_c, \\
I_2 &= N_a - 2N_b,
\end{aligned}
\tag{3}
$$

where I_2 is the imbalance between the number of atoms of type a and b. The total number of particles $N = N_a + N_b + 3N_c$ can be written using these conserved quantities,

$$
N = \frac{3I_1 - I_2}{2},
$$

and it is also conserved.

Writing the S-wave diagonal part of (2) as a combination of the conserved quantities (3) we find

$$
\alpha I_1^2 + \beta I_2^2 + \gamma I_1 I_2,
$$

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where we have used the following identification for the coupling constants

$$U_{aa} = \alpha + \beta + \gamma, \qquad U_{bb} = 4\beta, \qquad U_{cc} = 4\alpha,$$

$$U_{ab} = -4\beta - 2\gamma, \qquad U_{ac} = 4\alpha + 2\gamma, \qquad U_{bc} = -4\gamma.$$

Therefore the Hamiltonian (2) can also be written as

$$\begin{aligned} H = \ &\alpha I_1^2 + \beta I_2^2 + \gamma I_1 I_2 \\ &+ \mu_a N_a + \mu_b N_b + \mu_c N_c + \Omega(a^\dagger a^\dagger b^\dagger c + c^\dagger baa). \end{aligned} \tag{4}$$

This form will be used later when we show how the Hamiltonian (2) can be derived from a transfer matrix to establish integrability in the general context of the Yang-Baxter algebra.

2.1.2. Model for 3 different atoms: a, b and c

The Hamiltonian for a model of heterogeneous tri-atomic molecule labelled by d with one atom of type a, one atom of type b and one atom of type c is given by

$$\begin{aligned} H = \ &U_{aa}N_a^2 + U_{bb}N_b^2 + U_{cc}N_c^2 + U_{dd}N_d^2 \\ &+ U_{ab}N_aN_b + U_{ac}N_aN_c + U_{ad}N_aN_d + U_{bc}N_bN_c + U_{bd}N_bN_d + U_{cd}N_cN_d \\ &+ \mu_a N_a + \mu_b N_b + \mu_c N_c + \mu_d N_d + \Omega(a^\dagger b^\dagger c^\dagger d + d^\dagger cba). \end{aligned} \tag{5}$$

This Hamiltonian (5) has three independent conserved quantities,

$$\begin{aligned} I_1 &= N_a + N_d, \\ I_2 &= N_b + N_d, \\ I_3 &= N_c + N_d. \end{aligned} \tag{6}$$

The physical quantities representing the different imbalances between the number of atoms of different species (J_{ab}, J_{ac}, J_{bc}) and the total number of atoms N can be expressed as a combination of these quantities, for example,

$$\begin{aligned} J_{ab} &= N_a - N_b = I_1 - I_2, \\ J_{ac} &= N_a - N_c = I_1 - I_3, \\ J_{bc} &= N_b - N_c = I_2 - I_3, \\ N &= N_a + N_b + N_c + 3N_d = I_1 + I_2 + I_3, \end{aligned}$$

and are conserved as well.

We can write the S-wave diagonal part of the Hamiltonian (5) in terms of a combination of the independent conserved quantities (6) as

$$\alpha I_1^2 + \beta I_2^2 + \delta I_3^2 + \gamma I_1 I_2 + \rho I_1 I_3 + \theta I_2 I_3, \tag{7}$$

where the following identification has been made for the coupling constants

$$U_{aa} = \alpha, \qquad U_{bb} = \beta, \qquad U_{cc} = \delta, \qquad U_{dd} = \alpha + \beta + \delta + \gamma + \rho + \theta,$$

$$U_{ab} = \gamma, \qquad U_{ac} = \rho, \qquad U_{bc} = \theta, \qquad U_{bd} = 2\beta + \gamma + \theta, \qquad U_{cd} = 2\delta + \rho + \theta.$$

Then the Hamiltonian (5) can be also written as

$$H = \alpha I_1^2 + \beta I_2^2 + \delta I_3^2 + \gamma I_1 I_2 + \rho I_1 I_3 + \theta I_2 I_3$$
$$+ \mu_a N_a + \mu_b N_b + \mu_c N_c + \mu_d N_d + \Omega(a^\dagger b^\dagger c^\dagger d + d^\dagger cba). \tag{8}$$

2.2. Homonuclear-molecular model

In the homogeneous case, we can construct a model describing a triatomic-molecular BEC, where all atoms are identical.

2.2.1. Model for 3 atoms a

The Hamiltonian that describes the interconversion of a homogeneous triatomic molecule labelled by b with three atoms of type a is given by

$$H = U_{aa} N_a^2 + U_{bb} N_b^2 + U_{ab} N_a N_b + \mu_a N_a + \mu_b N_b$$
$$+ \Omega(a^\dagger a^\dagger a^\dagger b \, \alpha_-(N_a) + \alpha_-(N_a) b^\dagger aaa). \tag{9}$$

where $\alpha_-(N_a)$ is a function of N_a (see next section for more details) that controls the amplitude of interconversion Ω. This indicates that the density of atoms N_a has some influence in the generation of a bound-state composed by three identical atoms.

This Hamiltonian (9) has one conserved quantity,

$$I = N_a + 3N_b, \tag{10}$$

the total number of particles $N = N_a + 3N_b$.

3. Integrability and exact Bethe ansatz solution

In this section we will discuss the derivation, the integrability and the Bethe ansatz solution of these models. We begin with the $su(2)$-invariant R-matrix, depending on the spectral parameter u:

$$R(u) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & b(u) & c(u) & 0 \\ 0 & c(u) & b(u) & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

with $b(u) = u/(u + \eta)$ and $c(u) = \eta/(u + \eta)$. Above, η is an arbitrary parameter, to be chosen later. It is easy to check that $R(u)$ satisfies the Yang-Baxter equation

$$R_{12}(u - v)R_{13}(u)R_{23}(v) = R_{23}(v)R_{13}(u)R_{12}(u - v).$$

Here $R_{jk}(u)$ denotes the matrix acting non-trivially on the j-th and the k-th spaces and as the identity on the remaining space.

Next we define the Yang-Baxter algebra $T(u)$,

$$T(u) = \begin{pmatrix} A(u) & B(u) \\ C(u) & D(u) \end{pmatrix}$$

subject to the constraint

$$R_{12}(u - v)T_1(u)T_2(v) = T_2(v)T_1(u)R_{12}(u - v). \tag{11}$$

In what follows we will choose different realizations for the monodromy matrix $\pi(T(u)) = L(u)$ to obtain triatomic models for heteronuclear and homonuclear molecular BECs. In this construction, the Lax operators $L(u)$ have to satisfy the relation

$$R_{12}(u - v)L_1(u)L_2(v) = L_2(v)L_1(u)R_{12}(u - v). \tag{12}$$

Then, defining the transfer matrix, as usual, through

$$t(u) = tr\pi(T(u)) = \pi(A(u) + D(u)), \tag{13}$$

it follows from (11) that the transfer matrix commutes for different values of the spectral parameters; i. e., $[t(u), t(v)] = 0$. Consequently, the models derived from this transfer matrix will be integrable. Let us now particularize this construction for the hetero and homo-atomic molecular cases.

3.1. Heteronuclear-molecular models

We may choose the following realization for the two models of heteroatomic molecular BECs

$$\pi(T(u)) = L(u) = u^- G L^S(u^-) L^K(u^+), \tag{14}$$

with $u^\pm = u \pm \omega$, $G = diag(+, -)$, the Lax operator $L^S(u)$

$$L^S(u) = \frac{1}{u} \begin{pmatrix} u - \eta S^z & -\eta S^+ \\ -\eta S^- & u + \eta S^z \end{pmatrix}$$

in terms of the $su(2)$ Lie algebra with generators S^z and $S^\pm$ subject to the commutation relations

$$[S^z, S^\pm] = \pm S^\pm, \quad [S^+, S^-] = 2S^z,$$

and the Lax operator L^K

$$L^K(u) = \frac{1}{u} \begin{pmatrix} u + \eta K^z & \eta K^- \\ -\eta K^+ & u - \eta K^z \end{pmatrix},$$

in terms of the $su(1,1)$ Lie algebra with generators K^z and $K^\pm$ subject to the commutation relations

$$[K^z, K^\pm] = \pm K^\pm, \quad [K^+, K^-] = -2K^z. \tag{15}$$

Now, using two different realizations for the $su(2)$ and $su(1,1)$ algebras we will show how to construct the hetero-atomic Hamiltonians (2) and (5) from the transfer matrix (13) and present their exact Bethe ansatz solution.

3.1.1. Model for 2 atoms a and 1 atom b
Using the following realizations for the $su(2)$ and $su(1,1)$ algebras

$$S^+ = b^\dagger c, \quad S^- = c^\dagger b, \quad S^z = \frac{N_b - N_c}{2},$$

$$K^+ = \frac{(a^\dagger)^2}{2}, \quad K^- = \frac{(a)^2}{2}, \quad K^z = \frac{2N_a + 1}{4},$$

it is straightforward to check that the Hamiltonian (4) is related with the transfer matrix $t(u)$ (13) through

$$H = t(u) - \frac{1}{2}u^-\eta + \alpha I_1^2 + \beta I_2^2 + \delta I_1 I_2,$$

where the following identification has been made for the parameters

$$\mu_a = u^-\eta, \quad \mu_c = -\mu_b = u^+\eta, \quad \Omega = \frac{\eta^2}{2}.$$

We can apply the algebraic Bethe ansatz method, using as the pseudovacuum the product state ($|0\rangle = |k\rangle \otimes |\phi\rangle$, with $|k\rangle$ denoting the lowest weight state of the $su(1,1)$ algebra with weight k, i.e., $K^z|k\rangle = k|k\rangle$ and $|\phi\rangle$ denoting the highest weight state of the $su(2)$ algebra with weight m_z), to find the Bethe ansatz equations (BAE)

$$-\frac{(v_i - \omega - \eta m_z)(v_i + \omega + \eta k)}{(v_i - \omega + \eta m_z)(v_i + \omega - \eta k)} = \prod_{i \neq j}^{M} \frac{v_i - v_j - \eta}{v_i - v_j + \eta}, \quad i, j = 1, ..., M, \tag{16}$$

and the energies of the Hamiltonian (2) (see for example [7, 8])

$$E = (u^- - \eta m_z)(u^+ + \eta k) \prod_{i=1}^{M} \frac{u - v_i + \eta}{u - v_i}$$

$$- (u^- + \eta m_z)(u^+ - \eta k) \prod_{i=1}^{M} \frac{u - v_i - \eta}{u - v_i}$$

$$- \frac{1}{2}u^-\eta + \alpha I_1^2 + \beta I_2^2 + \gamma I_1 I_2. \tag{17}$$

3.1.2. Model for 3 different atoms: a, b and c

Using the following realizations for the $su(2)$ and $su(1,1)$ algebras

$$S^+ = c^\dagger d, \quad S^- = d^\dagger c, \quad S^z = \frac{N_c - N_d}{2},$$

$$K^+ = \frac{(a^\dagger b^\dagger)}{2}, \quad K^- = \frac{(ab)}{2}, \quad K^z = \frac{N_a + N_b + 1}{2},$$

it is straightforward to check that the Hamiltonian (8) is related with the transfer matrix $t(u)$ (13) through

$$H(u) = t(u) - u^- \eta + \alpha I_1^2 + \beta I_2^2 + \delta I_3^2 + \gamma I_1 I_2 + \rho I_1 I_3 + \theta I_2 I_3,$$

with the following identification for the parameters

$$\mu_a = \mu_b = u^- \eta, \quad \mu_c = -\mu_d = -u^+ \eta, \quad \Omega = \eta^2.$$

Applying the algebraic Bethe ansatz method we find the Bethe ansatz equations (BAE)

$$-\frac{(v_i - \omega - \eta m_z)(v_i + \omega + \eta k)}{(v_i - \omega + \eta m_z)(v_i + \omega - \eta k)} = \prod_{i \neq j}^{M} \frac{v_i - v_j - \eta}{v_i - v_j + \eta}, \quad i,j = 1, ..., M, \quad (18)$$

and the energies of the Hamiltonian (5)

$$E = (u^- - \eta m_z)(u^+ + \eta k) \prod_{i=1}^{M} \frac{u - v_i + \eta}{u - v_i}$$

$$- (u^- + \eta m_z)(u^+ - \eta k) \prod_{i=1}^{M} \frac{u - v_i - \eta}{u - v_i}$$

$$- u^- \eta + \alpha I_1^2 + \beta I_2^2 + \delta I_3^2 + \gamma I_1 I_2 + \rho I_1 I_3 + \theta I_2 I_3. \quad (19)$$

3.2. Homonuclear-molecular model

In this case we may choose the following realization for the Yang-Baxter algebra

$$\pi(T(u)) = L(u) = \eta^{-1} G L^b(u - \delta - \eta^{-1}) L^A(u + \omega), \quad (20)$$

with, $G = diag(-, +)$, the Lax operator $L^b(u)$

$$L^b(u) = \begin{pmatrix} u + \eta N_b & b \\ b^\dagger & \eta^{-1} \end{pmatrix}$$

in terms of the canonical boson operators b and $b^\dagger$ with $N_b = b^\dagger b$, subject to the commutation relations

$$[b, b] = [b^\dagger, b^\dagger] = 0, \quad [b, b^\dagger] = I,$$

and the Lax operator L^A

$$
L^A(u) = \begin{pmatrix} u + \frac{\eta}{2}A_0 & \eta A_- \\ -\eta A_+ & u - \frac{\eta}{2}A_0 \end{pmatrix},
$$

in terms of the $sl(2)$ Lie algebra with generators A_0 and $A_\pm$, subject to the commutation relations

$$
[A_-, A_+] = A_0, \quad [A_0, A_\pm] = \pm 2A_\pm. \tag{21}
$$

We find from the L operator (20) the following transfer matrix

$$
t(u) = -\eta^{-1}(u + \omega + \frac{\eta}{2}A_0)(u - \delta - \eta^{-1} + \eta N_b)
$$
$$
+ \eta^{-2}(u + \omega - \frac{\eta}{2}A_0) + bA_+ + b^\dagger A_-, \tag{22}
$$

with

$$
t(0) = \eta^{-1}\omega(\delta + 2\eta^{-1}) - \omega N_b + \frac{1}{2}(\delta - \eta N_b)A_0 + bA_+ + b^\dagger A_-. \tag{23}
$$

There is a one-mode realization of the $sl(2)$ algebra [18]

$$
A_0 = \alpha_0(N), \quad A_- = \alpha_-(N)a^l, \quad A_+ = (a^\dagger)^l \alpha_-(N)
$$

with

$$
\alpha_0(N) = \frac{2}{l}(N - R) + \alpha_0(R) \tag{24}
$$

$$
\alpha_-(N) = \sqrt{\frac{N!}{(N+l)!}(\frac{1}{l}(N - R) + \alpha_0(R))(\frac{1}{l}(N - R) + 1)} \tag{25}
$$

where $N = a^\dagger a$ and $l \in \mathbb{N}$. The operator R is

$$
R = \begin{cases} 0, & if \quad l = 1 \\ \dfrac{l-1}{2} + \displaystyle\sum_{m=1}^{l-1} \dfrac{e^{-(2\pi m/l)N}}{e^{(2\pi m/l)} - 1}, & if \quad l > 1 \end{cases}
$$

and acts on the states $\{|n\rangle\}$ as $R|n\rangle = n \bmod l|n\rangle$. The function $\alpha_0(R)$ is a function of the spectrum of R. For $n = r < l$, we have

$$
\frac{1}{l}(N - R)|r\rangle = 0|r\rangle \tag{26}
$$

with $A_0 = \alpha_0(R)$ such that $\alpha_0(R)|r\rangle = \alpha_0(r)|r\rangle$ and $R|r\rangle = r|r\rangle$. The operator R commutes with a^l and $(a^\dagger)^l$ and so is a conserved quantity for all models presented in this paper.

Now we will apply this realization to show how to construct the Hamiltonian (9) from the transfer matrix (22) and present their exact Bethe ansatz solution. For $l = 3$,

which is the case of interest here, it is straightforward to check that the Hamiltonian (9) is related with the transfer matrix $t(0)$ (23) through

$$H = t(0) \qquad (27)$$

where we have the following identification

$$\eta = 9U_a + U_b - 3U_{ab}$$

$$6(\omega + \delta) = (18U_a - 2U_b)N - \eta\rho + 18\mu_a - 6\mu_b$$

$$36\eta^{-1}\omega\delta + 72\omega\eta^{-2} = \eta\rho^2 + [(4U_b - 6U_{ab})N + 6(\mu_b - 3\mu_a + \omega)]\rho$$
$$+ 4U_bN^2 + 12(\mu_b + \omega)N$$

with $\rho \equiv \rho(R) = 3\alpha_0(R) - 2R$. Let $|0\rangle_b$ denotes the Fock vacuum state and let $|r\rangle_A$ denotes the lowest weight state of the $sl(2)$ algebra where $r = 0$, 1, 2, are the eingenvalues of R for $l = 3$ and $N = nl + r$, with $n \in N$. On the product state $|\Psi\rangle = |r\rangle_A \otimes |0\rangle_b$ we can apply the algebraic Bethe ansatz method to find the Bethe ansatz equations (BAE)

$$\frac{(1 - \eta v_i + \eta\delta)(v_i + \omega + \frac{\eta}{2}\alpha_0(r))}{v_i + \omega - \frac{\eta}{2}\alpha_0(r)} = \prod_{i \neq j}^{M} \frac{v_i - v_j - \eta}{v_i - v_j + \eta}, \quad i, j = 1, ..., M, \quad (28)$$

and the energies of the Hamiltonian (2)

$$E = \eta^{-1}(\delta + \eta^{-1})\left(\omega + \frac{\eta}{2}\alpha_0(r)\right)\prod_{i=1}^{M}\frac{v_i - \eta}{v_i}$$
$$+ \eta^{-2}\left(\omega - \frac{\eta}{2}\alpha_0(r)\right)\prod_{i=1}^{M}\frac{v_i + \eta}{v_i}. \qquad (29)$$

4. Summary

We have introduced three new integrable models for both, homogeneous and heterogeneous tri-atomic molecular BECs obtained through a combination of Lax operators constructed using special realizations of the $su(2)$ and $su(1,1)$ algebras and a particular one-mode multibosonic representation of $sl(2)$, possibilities that were overlooked in previous studies. The models were solved by means of the algebraic Bethe ansatz method and their corresponding energies and Bethe ansatz equations were derived.

Acknowledgments

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