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Bosonic realisation of sp(4, R) and the spectrum of two-particle quantum systems

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Abstract. A new bosonic Holstein-Primakoff-type realisation of sp(4,R) is applied in the development of '1/N' expansions of non-relativistic spin-independent two-particle Hamiltonians. As a non-trivial example, the spectrum of helium-like ions is considered and the energies of the low-lying levels with given values of total angular momentum are computed. The calculation is explicitly performed in an approximation up to the second degree in the small expansion parameter.

1. Introduction

The relevance of the non-compact real symplectic Lie algebras sp(2d, R) in the study of the non-relativistic spin-independent many-particle quantum systems is widely recognised after the works of Mlodinow and Papanicolaou [1, 2]. These authors first introduced a Holstein-Primakoff-type [3] realisation of the irreducible representations of the algebras mentioned. In [1] the case d = 1 was fully analysed. The case d = 2was partially developed in [2], where the representations associated with zero angular momentum states of two-particle systems were considered. During the subsequent years, much work was done in obtaining bosonic realisations for the more general cases, and new physical applications were proposed [4-7].

In the present paper, the method of Mlodinow and Papanicolaou will be extended in order to include states with arbitrary angular momentum of two-particle quantum systems. It will be done on the basis of a new bosonic Holstein-Primakoff-type realisation of the representations of sp(4, R) associated with given values L of the total angular momentum. This realisation was recently obtained by the present author [8]. Other realisations accessible from the literature are not appropriate for the mentioned extension due to the lack of analyticity and explicitness.

The general formulation is developed in § 2. As a non-trivial application, the non-relativistic Hamiltonian of helium-like ions is considered in § 3. There, the energy of the low-lying states with given angular momentum L are computed in an approximation which includes the second order in the small expansion parameter. Some remarks of general order are mentioned in the conclusions. For convenience, many of the formulae are presented in the appendices.

2. The '1/N' expansion

The present approach can be applied to every non-relativistic spin-independent twoparticle quantum system with a rotationally invariant Hamiltonian. However, it will be enough to consider the sufficiently typical and interesting class of Hamiltonians proposed by Mlodinow and Papanicolaou [2]:

$$H = \frac{1}{4}(p^{2} + P^{2}) + 2\nu g^{2}[(r^{2} + R^{2} + 2r \cdot R)^{\nu} + (r^{2} + R^{2} - 2r \cdot R)^{\nu}] - 2\nu e^{2}(4r^{2})^{\nu}$$
(1)
where

$$r = \frac{1}{2}(r_1 - r_2) \qquad R = \frac{1}{2}(r_1 + r_2) p = p_1 - p_2 \qquad P = p_1 + p_2$$
(2)

are the centre-of-mass coordinates of the two interacting particles, which have equal masses normalised to unity. The parameters g, e, ν , as well as the space dimension N, are taken to be arbitrary for the moment. For physical space N = 3.

Let us introduce the operators

$$\eta_{1t} = \left(\frac{\omega}{2}\right)^{1/2} x_t - i\left(\frac{1}{2\omega}\right)^{1/2} p_t \qquad \xi_{1t} = \left(\frac{\omega}{2}\right)^{1/2} x_t + i\left(\frac{1}{2\omega}\right)^{1/2} p_t \eta_{2t} = \left(\frac{\Omega}{2}\right)^{1/2} X_t - i\left(\frac{1}{2\Omega}\right)^{1/2} P_t \qquad \xi_{2t} = \left(\frac{\Omega}{2}\right)^{1/2} X_t + i\left(\frac{1}{2\Omega}\right)^{1/2} P_t$$
(3)

which are the creation and annihilation operators of an auxiliary set of harmonic oscillators, associated with the Schrödinger operators (2). The parameters ω and Ω will be determined below.

As is well known, due to the Bose commutations relation between the operators η_{it} and ξ_{it} , i = 1, 2, t = 1, 2, ..., N, the following operators generate the Lie algebra sp(4, R):

$$C_{ij} = \sum_{t=1}^{N} \eta_{it} \xi_{jt} + \frac{1}{2} N \delta_{ij}$$

$$B_{ij}^{+} = \sum_{t=1}^{N} \eta_{it} \eta_{jt} \qquad B_{ij} = \sum_{t=1}^{N} \xi_{it} \xi_{jt}.$$
(4)

Using the identities

$$p^{2} = \omega (C_{11} - \frac{1}{2}B_{11} - \frac{1}{2}B_{11}^{+}) \qquad P^{2} = \Omega (C_{22} - \frac{1}{2}B_{22} - \frac{1}{2}B_{22}^{+})$$

$$r^{2} = \omega^{-1} (C_{11} + \frac{1}{2}B_{11} + \frac{1}{2}B_{11}^{+}) \qquad R^{2} = \Omega^{-1} (C_{22} + \frac{1}{2}B_{22} + \frac{1}{2}B_{22}^{+}) \qquad (5)$$

$$2r \cdot R = (\omega \Omega)^{-1/2} (C_{12} + C_{21} + B_{12} + B_{12}^{+})$$

the Hamiltonians (1) can be written as a function of the sp(4, R) generators.

The states with fixed angular momentum L span a basis of an irreducible representation of sp(4, R), as was shown by Moshinsky and Quesne [9, 10] applying their notion of complementarity of Lie groups to the chain $Sp(4N, R) \supset Sp(4, R) \times O(N)$. In fact, computing the second-order Casimir invariant of Sp(4, R) with generators (4), it follows that [2, 11]

$$L(L+N-2) = 2s(s+1) + 2q(q-3) - \frac{1}{2}N(N-6).$$
(6)

Here, L(L+N-2) are the eigenvalues of the angular momentum operator L^2 (in N dimensions) and s, q are the parameters introduced by Evans [12] in order to classify the irreducible representations of so(3, 2) ~ sp(4, R) in a separable Hilbert space.

From (6), a systematic account of the irreps with given values L of angular momentum can be obtained choosing

$$s = \frac{1}{2}L$$
 $q = s + \frac{1}{2}N = \frac{1}{2}(N + L).$ (7)

If $N \ge 3$, such values of parameters s, q belong to one of the discrete series discussed by Evans. The bosonic realisation of this series of irreps was given in [8] and is reproduced in appendix 1 for completeness. Here it can only be mentioned that the representation space is spanned by the state vectors

$$|\nu_1, \nu_2, l\rangle \otimes |s, \delta\rangle$$
 (8)

where $\{|\nu_1, \nu_2, l\rangle, \nu_1, \nu_2, l = 0, 1, 2, ...\}$ is an orthonormal basis for the Weyl algebra w(3), prametrised by the eigenvalues of the occupation number operators $N_a = b_a^+ b_a$, a = 1, 2, 3, of three independent bosonic oscillators, and $\{|s, \delta\rangle, \delta = -s, -s + 1, ..., s\}$ is a standard basis of su(2), whose generators will be denoted by S_1, S_2, S_3 . On such a space the operators (5) can be put in the form

$$p^{2} = \omega(b_{1} - q_{1})(b_{1}^{+} - q_{1}) \qquad P^{2} = \Omega(b_{2} - q_{2})(b_{2}^{+} - q_{2})$$

$$r^{2} = \omega^{-1}(b_{1} + q_{1})(b_{1}^{+} + q_{1}) \qquad R^{2} = \Omega^{-1}(b_{2} + q_{2})(b_{2}^{+} + q_{2}) \qquad (9)$$

$$2r \cdot R = (\omega\Omega)^{-1/2}(b_{1} + q_{1})[(b_{2} + q_{2})b_{3}^{+}F + S_{+}(b_{2}^{+} + q_{2})G] + HC$$

where HC stands for Hermitian conjugation, $S_{\pm} = S_1 \pm iS_2$, and the Hermitian operators q_1 , q_2 , F, G, are given in appendix 1, where their explicit dependence on parameter q can be seen.

Now, introducing the realisation (9) in the Hamiltonian (1), an expansion in powers of parameter $x \equiv q^{-1/2} = [2/(N+L)]^{1/2}$ can be performed:

$$H = x^{-2}H^{(-2)} + x^{-1}H^{(-1)} + H^{(0)} + xH^{(1)} + x^{2}H^{(2)} + \dots$$
(10)

The operator $H^{(-1)}$ comes out linear in the operators $b_1 + b_1^+$ and $b_2 + b_2^+$ and can be set equal to zero with the choice of parameters ω , Ω as the positive solutions of the algebraic equations

$$\Omega^{2} = 16\nu\bar{g}^{2}\left(\frac{1}{\omega} + \frac{1}{\Omega}\right)^{\nu-1} \qquad \Omega^{2} - \omega^{2} = 32\nu^{2}\bar{e}^{2}\left(\frac{4}{\omega}\right)^{\nu-1}$$
(11)

where the rescaled parameters $\bar{g}^2 = g^2 x^{2(1-\nu)}$, $\bar{e}^2 = e^2 x^{2(1-\nu)}$ were introduced. Up to the redefinition of the expansion parameter this result was given by Mlodinow and Papanicolaou [2]. With this choice of ω and Ω , the leading term becomes

$$H^{(-2)} = (\omega + \Omega)(1 + \nu)/4\nu$$
(12)

and the following 'Gaussian' approximation is

$$H^{(0)} = H_{12} + H_3 + \frac{1}{4}(\omega - \Omega)S_3$$
(13)

where

$$H_{12} = \omega b_1^+ b_1 + \Omega b_2^+ b_2 + K_1 (b_1 + b_1^+)^2 + K_2 (b_2 + b_2^+)^2 + K_{12} (b_1 + b_1^+) (b_2 + b_2^+)$$
(14)

$$H_3 = \varepsilon b_3^+ b_3 + K_3 (b_3 + b_3^+)^2 \tag{15}$$

and

$$K_{1} = (\nu - 1)(\omega^{2} + \omega\Omega - \Omega^{2})/8(\omega + \Omega)$$

$$K_{2} = (\nu - 1)\omega\Omega/8(\omega + \Omega)$$

$$K_{12} = K_{3} = (\nu - 1)\Omega^{2}/4(\omega + \Omega)$$

$$\varepsilon = (\omega + \Omega)/2.$$
(16)

The following two terms $H^{(1)}$, $H^{(2)}$ are given in appendix 2 and will be used in the computation of the first non-trivial correction to the 'Gaussian' approximation.

The diagonalisation of $H^{(0)}$ is straightforward by means of a canonical transformation b_1 , b_2 , $b_3 \rightarrow \alpha$, β , γ , which, for completeness, is given in appendix 3. Now the Hamiltonian is transformed to

$$H = E_{0L} + \lambda_1 \alpha^+ \alpha + \lambda_2 \beta^+ \beta + \lambda_3 \gamma^+ \gamma + \frac{1}{2} (\omega - \Omega) (S_3 - s) + x H^{(1)} + x^2 H^{(2)} + \dots$$
(17)

where E_{0L} is the 'Gaussian' approximation to the energy of the low-lying level with given angular momentum L, represented (in this approximation) by the state $|0, 0, 0\rangle \otimes |s, s\rangle$, s = L/2,

$$E_{0L} = \frac{(\omega + \Omega)(1 + \nu)}{4x^2\nu} + \frac{1}{2}(\lambda_1 + \lambda_2 + \lambda_3) - \frac{3}{4}(\omega + \Omega) + \frac{1}{2}(\omega - \Omega)s.$$
(18)

The values of the frequencies λ_1 , λ_2 , λ_3 are those given by Mlodinow and Papanicolaou [2]:

$$\lambda_{1,2}^{2} = \frac{1}{2} [\Omega(\Omega + 4K_{2}) + \omega(\omega + 4K_{1}) \mp \Delta^{1/2}]$$

$$\lambda_{3}^{2} = \varepsilon(\varepsilon + 4K_{3})$$

$$\Delta = [\Omega(\Omega + 4K_{2}) - \omega(\omega + 4K_{1})]^{2} + 16\omega\Omega K_{12}^{2}.$$
(19)

The first correction to the 'Gaussian' approximation is obtained with the effective Hamiltonian

$$H_{\rm eff} = H_0 + x(H^{(1)} + xH^{(2)})$$
(20)

where $H_0 \equiv x^{-2}H^{(-2)} + H^{(0)}$, and all the operators are transformed to the new variables α , β , γ . Then the perturbative theory must be applied up to the second order in the small parameter x, giving

$$E_{L} = E_{0L} + x^{2} \left(\sum_{E \neq E_{0L}} \frac{|\langle E|H^{(1)}|E_{0L}\rangle|^{2}}{E_{0L} - E} + \langle E_{0L}|H^{(2)}|E_{0L}\rangle \right)$$
(21)

for the energies of the low-lying states with angular momentum L. Here $|E\rangle$ are the eigenstates of H_0 . In particular, $|E_{0L}\rangle = |0, 0, 0\rangle \otimes |s, s\rangle$.

In the following section, for the particular case of helium-like ions, the explicit calculation of these energies is presented. For the other excited states the computation can be realised in a similar manner. Further, and more realistic, approximations could require more complicated iterative computation, but as direct as discussed in this paper.

3. Low-lying levels of helium-like ions

With the choice $\nu = -\frac{1}{2}$, the Hamiltonian (1) describes the non-relativistic behaviour of helium-like ions. In atomic units ($e^2 = 1$) the rescaled coupling constants become

$$\bar{g}^2 = Z \left(\frac{2}{N+L}\right)^{3/2} \qquad \bar{e}^2 = \left(\frac{2}{N+L}\right)^{3/2}$$
(22)

where Z is the strength of nuclear charge. As was shown by Mlodinow and Papanicolaou, the unique positive solution of (11) is

$$\omega = \left(\frac{2}{N+L}\right)^{3} \eta \qquad \Omega = \left(\frac{2}{N+L}\right)^{3} H$$

$$\eta = [\alpha(\alpha-2)]^{-2} \qquad H = (\alpha-1)[\alpha(\alpha-2)]^{-2}$$

$$\alpha = [64Z^{2} - 1 + (1 + 128Z^{2})^{1/2}]/2(16Z^{2} - 1).$$
(23)

Rescaling the frequencies λ_1 , λ_2 , λ_3 as

$$\lambda_i = \left(\frac{2}{N+L}\right)^3 \eta_i \qquad i = 1, 2, 3 \tag{24}$$

the effective Hamiltonian (20) takes the form

$$H = E_{0L} + \left(\frac{2}{N+L}\right)^{3} \left[\eta_{1}\alpha^{+}\alpha + \eta_{2}\beta^{+}\beta + \eta_{3}\gamma^{+}\gamma - \frac{1}{2}(H-\eta)(S_{3}-s) + \left(\frac{2}{N+L}\right)^{1/2}h^{(1)} + \left(\frac{2}{N+L}\right)h^{(2)}\right]$$
(25)

where s = L/2,

$$E_{0L} = -\left(\frac{2}{N+L}\right)^{3} \left[\left(\frac{H+\eta}{4}\right) \left(\frac{N+L}{2}\right) + \frac{3}{4}(H+\eta) - \frac{1}{2}(\eta_{1}+\eta_{2}+\eta_{3}) + \frac{1}{4}(H-\eta)L \right]$$
(26)

and $h^{(1)}$, $h^{(2)}$ have the same form as $H^{(1)}$, $H^{(2)}$ but the parameters ω , Ω , λ_1 , λ_2 , λ_3 were replaced by η , H, η_1 , η_2 , η_3 .

The computation of the energies using (21) gives, for Z = 2, 3, ..., 8, the values

$$E_{L} = -\left(\frac{2}{N+L}\right)^{3} \left[T_{1}\left(\frac{N+L}{2}\right) + T_{2} + T_{3}L + \left(\frac{2}{N+L}\right)(T_{4} + T_{5}L + T_{6}L^{2})\right]$$
(27)

with the quantities T_1, \ldots, T_6 presented in table 1.

Setting N = 3, the expression (27) corresponds to the energies of the low-lying states of the helium-like ions in each angular momentum sector, in an approximation of the second order in the small expansion parameter $[2/(3+L)]^{1/2}$. For L = 0 the numerical values coincide exactly with those given by Mlodinow and Papanicolaou [2].

Ζ	T_1	<i>T</i> ₂	T ₃	T_4	T ₅	<i>T</i> ₆
2	2.7378	3.0288	0.2529	2.2155	4.6346	-0.0724
3	7.0321	7.4477	0.4268	5.5896	8.5463	-0.1353
4	13.3257	13.8712	0.6021	10.4389	14.1634	-0.1999
5	21.6190	22.2958	0.7780	16.7831	21.3250	-0.2652
5	31.9122	32.7208	0.9542	24.6255	30.0036	-0.3308
7	44.2053	45.1460	1.1305	33.9670	40.1905	-0.3966
8	58.4984	59.5712	1.3070	44.8081	51.8821	-0.4626

Table 1. Numerical values in the expression of the energies E_L for He-like ions.

4. Conclusions

The expansion method based in the application of the bosonic realisation of sp(4, R) can, in principle, be developed for Hamiltonians which are arbitrary functions of the rotational invariants (5). In the particular cases considered above, the first few terms give a relatively good approximation for the low-lying states in each angular momentum sector. More accurate results, and the extension to other excited states, require the consideration of additional terms of the expansion. The same could also be desirable for the analysis of the convergence problem.

Extensions to more complex systems, with say three or more particles, could be developed on the basis of the representation of more general Lie algebras sp(2d, R). However, to the best of my knowledge, explicit and analytic realisations of these algebras are not available at the present. The known results require numerical computation at some stage.

Appendix 1. Bosonic Holstein-Primakoff-type realisation of sp(4, R)

In the following $N_a \equiv b_a^+ b_a$, a = 1, 2, 3, are the occupation number operators of three independent bosonic oscillators, and S_1 , S_2 , S_3 are the generators of a su(2) algebra, $S_1^2 + S_2^2 + S_3^2 = s(s+1)$.

$$C_{11} = q + 2N_1 + N_3 + S_3$$
 $C_{22} = q + 2N_2 + N_3 - S_3$ (A1.1)

$$C_{12} = q_1 b_2 b_3^+ F + F b_3 b_1^+ q_2 + q_1 S_+ q_2 G + G b_1^+ b_2 S_-$$
(A1.2)

$$B_{11} = 2b_1q_1 \qquad B_{22} = 2b_2q_2 \tag{A1.3}$$

$$B_{12} = b_1 b_2 b_3^+ F + F b_3 q_1 q_2 + b_1 S_+ q_2 G + G b_2 S_- q_1$$
(A1.4)

where $S_{\pm} = S_1 \bullet iS_2$ and

$$q_1 \equiv (q + N_1 + N_3 + S_3 - 1)^{1/2}$$
 $q_2 \equiv (q + N_2 + N_3 - S_3 - 1)^{1/2}$ (A1.5)

$$F = \left(\frac{(q+S+N_3)(q-s+N_3-1)(2q+N_3-2)}{(q+N_3+S_3)(q+N_3+S_3-1)(q+N_3-S_3)(q+N_3-S_3-1)}\right)^{1/2}$$
(A1.6)

$$G = \left(\frac{(q - S_3 - 2)(q + S_3 - 1)}{(q + N_3 + S_3)(q + N_3 + S_3 - 1)(q + N_3 - S_3 - 1)(q + N_3 - S_3 - 2)}\right)^{1/2}.$$
 (A1.7)

The remaining operators follow by Hermitian conjugation.

Appendix 2. The Gaussian corrections $H^{(1)}$, $H^{(2)}$

The following operators are given as functions of the original variables b_1 , b_2 , b_3 , as they appear in the expansion (10):

$$H^{(1)} = 2c_1(A_+B_+ + A_-B_-) + 2c_2(A_+^3 + A_-^3) + 2d_1A_0B_0 + d_2A_0^3$$

$$H^{(2)} = c_1(B_+^2 + B_-^2 + 2A_+C_+ + 2A_-C_-) + 3c_2(A_+^2B_+ + A_-^2B_-) + c_3(A_+^4 + A_-^4)$$
(A2.1)

$$+ d_1(B_0^2 + 2A_0C_0) + 3d_2A_0^2B_0 + d_3A_0^4$$
(A2.2)

where the complete symmetrisation of the products of non-commuting operators A_m , B_m , m = +, -, 0, must be performed. These operators are defined as follows:

$$A_0 = b_1 + b_1^+ \qquad B_0 = 2N_1 + N_3 + S_3 \qquad C_0 = \frac{1}{2}b_1(N_1 + N_3 + S_3 - 1)$$
(A2.3)

$$A_{\pm} = V \pm W$$
 $B_{\pm} = X \pm Y$ $C_{\pm} = Z \pm T$ (A2.4)

$$V = \omega^{-1}(b_1 + b_1^+) + \Omega^{-1}(b_2 + b_2^+)$$
(A2.5)

$$W = (2/\omega\Omega)^{1/2}(b_3 + b_3^+)$$
(A2.6)

$$X = \omega^{-1}(2N_1 + N_3 + S_3) + \Omega^{-1}(2N_2 + N_3 - S_3)$$
(A2.7)

$$Y = (2/\omega\Omega)^{1/2}(b_1 + b_2)b_3^+ + (\omega\Omega)^{-1/2}S_+ + HC$$
(A2.8)

$$Z = (2\omega)^{-1}b_1(N_1 + N_3 + S_3 - 1) + (2\Omega)^{-1}b_2(N_2 + N_3 - S_3 - 1) + \text{HC}$$
(A2.9)

$$T = (8\omega\Omega)^{-1/2}b_3(2N_1 + 2N_2 + N_3 + 4b_1^+b_2^+ - 1) + (\omega\Omega)^{-1/2}(b_1 + b_2^+)S_+ + \text{HC.}$$
(A2.10)

Here HC stands for hermitian conjugate.

The constant coefficients c_n , d_n , n = 1, 2, 3, are given by

$$c_n = \frac{\Gamma(\nu)\Omega^{2+n}\omega^n}{8\Gamma(\nu-n)\Gamma(2+n)(\omega+\Omega)^n} \qquad d_n = \frac{\Gamma(\nu)(\omega^2 - \Omega^2)}{4\Gamma(\nu-n)\Gamma(2+n)\omega}.$$
 (A2.11)

Appendix 3. Canonical transformation which diagonalises $H_{12} + H_3$

$$\binom{b_1}{b_2} = F^{(+)}\binom{\alpha}{\beta} + F^{(-)}\binom{\alpha^+}{\beta^+}$$
(A3.1)

where the 2×2 real matrices $F^{(\pm)}$ are defined as follows:

$$F_{ij}^{(\pm)} = \frac{1}{2} D_{ij} \theta_{ij}^{(\pm)} \qquad i, j = 1, 2 \text{ (no summation)}$$
(A3.2)

$$\theta_{ij}^{(\pm)} = \begin{pmatrix} \left(\frac{\omega}{\lambda_1}\right)^{1/2} \pm \left(\frac{\lambda_1}{\omega}\right)^{1/2} & \left(\frac{\omega}{\lambda_2}\right)^{1/2} \pm \left(\frac{\lambda_2}{\omega}\right)^{1/2} \\ \left(\frac{\Omega}{\lambda_1}\right)^{1/2} \pm \left(\frac{\lambda_1}{\Omega}\right)^{1/2} & \left(\frac{\Omega}{\lambda_2}\right)^{1/2} \pm \left(\frac{\lambda_2}{\Omega}\right)^{1/2} \end{pmatrix}$$
(A3.3)

$$D_{ij} = (\Delta_{11}^2 + \Delta_{12}^2)^{-1/2} \Delta_{ij}$$
(A3.4)

$$\Delta_{11} = -\Delta_{22} = \frac{1}{2} [\Omega(\Omega + 4K_2) - \omega(\omega + 4K_1) + \Delta^{1/2}]$$
(A3.5)

$$\Delta_{12} = -2(\omega \Omega)^{1/2} K_{12} \tag{A3.6}$$

$$b_3 = G^{(+)}\gamma + G^{(-)}\gamma^+ \tag{A3.7}$$

$$G^{(\pm)} = \frac{1}{2} \left[\left(\frac{\varepsilon}{\lambda_3} \right)^{1/2} \pm \left(\frac{\lambda_3}{\varepsilon} \right)^{1/2} \right].$$
(A3.8)

The parameters ω , Ω , K_1 , K_2 , K_{12} , ε , λ_1 , λ_2 , λ_3 and Δ were defined in (11), (16) and (19).

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