sp(4) S.G.A. for a large class of three-body problems

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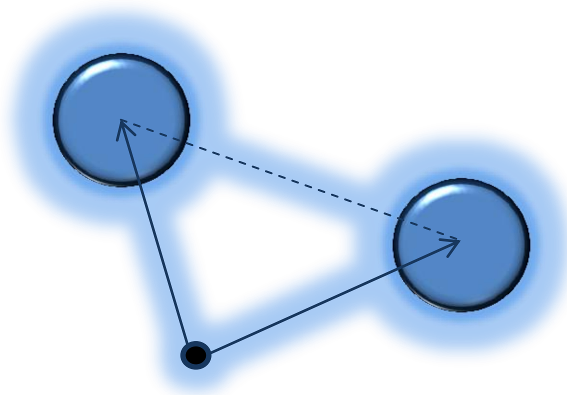
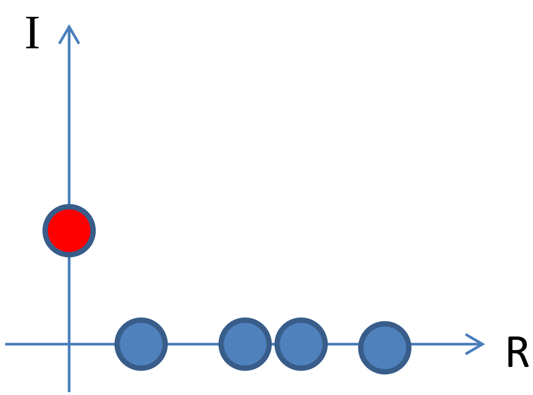




Iachello's students complex plane

Connections with you and an illuminated quotation!

- Arima -> necessity of simple models
- Leviatan -> partial «solvability»
- Wolf -> symplectic (and non-compact) has important solutions, many of which are still lacking applications
- Dukelsky, Kirchbach, Garcia-Ramos -> mentioned su(1,1)
- Draayer -> uses symplectic, mentioned both Rowe and Bahri
- Vitturi -> 1D three-body models are excersises for students (gosh, I'm one of his students). BUT 3D is difficult...

LIPKIN'S BOOK: «Phases, a perennial headache»

Personal history of this work

- 2002: fundamental work by Rowe and Bahri, JPA 31 (1998) 4947-4961
- 2003-2010: Used sp(2) techniques to solve Bohr hamiltonian with Coulomb and Kratzer potentials and a variety of other potentials (Iachello docet)
- 2004 (while in Belgium): got the idea to extend to two coordinates ->sp(4)
- 2005-2006: tried to calculate matrix elements following E. De Souza Bernardes and failed... (but with finite dim. rep. !)
- 2007: talked with Rowe in Seattle and he said: «Could you formulate your idea in mathematical terms? »
- 2011: at the ECT* discussions with W.de Graaf (Univ. Trento) on finite dimensional representations of sp(4)
- 2012: finally understood the infinite dimensional representations of sp(4) and found an easy way to calculate matrix elements by generalizing a method that is contained in Wybourne's book!

2Body: Rowe –Bahri JPA 31 (1998) 4947-4961

Infinitesimal generators of Sp(1, ℝ) are given by

$$[\hat{x}_j, \hat{p}_k] = i\hbar\delta_{jk}\hat{I}.$$

$$\hat{Z}_1 = p^2 = \sum_i p_i^2 \qquad \hat{Z}_2 = r^2 = \sum_i x_i^2$$

$$\hat{Z}_3 = \tfrac{1}{2}(r\cdot p + p\cdot r) = \tfrac{1}{2}\sum_i (x_i p_i + p_i x_i)$$

$$[\hat{Z}_1, \hat{Z}_2] = -4i\hbar\hat{Z}_3 \qquad [\hat{Z}_3, \hat{Z}_1] = 2i\hbar\hat{Z}_1$$

$$[\hat{Z}_3, \hat{Z}_2] = -2i\hbar\hat{Z}_2.$$

$$\hat{X}_1 = \frac{1}{4\hbar}\left(\hat{Z}_1 - \hat{Z}_2\right)$$

$$\hat{X}_2 = \frac{1}{2\hbar}\hat{Z}_3 \qquad \hat{X}_3 = \frac{1}{4\hbar}\left(\hat{Z}_1 + \hat{Z}_2\right)$$

$$[\hat{X}_1, \hat{X}_2] = -i\hbar\hat{X}_3 \qquad [\hat{X}_2, \hat{X}_3] = i\hbar\hat{X}_1$$

$$[\hat{X}_3, \hat{X}_1] = i\hbar\hat{X}_2.$$

$\mathfrak{su}(1, 1)$

$$\hat{X}_\pm = \hat{X}_1 \pm i\hat{X}_2 \qquad \hat{X}_0 = \hat{X}_3$$

$$[\hat{X}_-, \hat{X}_+] = 2\hat{X}_0 \qquad [\hat{X}_0, \hat{X}_\pm] = \pm\hat{X}_\pm$$

Rowe –Bahri continued

Positive discrete series irreps for $\mathfrak{su}(1,1)$ are characterized by a lowest weight λ with positive real values. Orthonormal bases for these irreps are given by states $\{|n\lambda\rangle; n = 0, 1, 2, \ldots\}$ which satisfy the equations

$$\hat{X}_+|n\lambda\rangle = \sqrt{(\lambda+n)(n+1)}|n+1,\lambda\rangle$$
$$\hat{X}_-|n+1,\lambda\rangle = \sqrt{(\lambda+n)(n+1)}|n\lambda\rangle$$
$$\hat{X}_0|n\lambda\rangle = \tfrac{1}{2}(\lambda+2n)|n\lambda\rangle$$

$$\lambda = \ell + dim/2$$

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2\left(r^2 + \frac{\varepsilon}{r^2}\right)$$

$$E_{nl} = \left[2n + 1 + \sqrt{(l+\tfrac{1}{2})^2 + \varepsilon}\right]\hbar\omega. \qquad \text{3D}$$

$$H_\varepsilon = \frac{1}{2}\hbar\omega\left(-\nabla^2 + \beta^2 + \frac{\varepsilon}{\beta^2}\right)$$

$$E_{nv}(\varepsilon) = \left[2n + 1 + \sqrt{(v+\tfrac{3}{2})^2 + \varepsilon}\right]\hbar\omega. \qquad \text{5D}$$

Davidson potential in both cases

Example: quartic potential

$$\hat{X}_+|n\lambda\rangle = \sqrt{(\lambda+n)(n+1)}|n+1,\lambda\rangle$$
$$\hat{X}_-|n+1,\lambda\rangle = \sqrt{(\lambda+n)(n+1)}|n\lambda\rangle$$
$$\hat{X}_0|n\lambda\rangle = \tfrac{1}{2}(\lambda+2n)|n\lambda\rangle$$

$$\mathcal{Z}_{1mn} = \langle m\lambda \mid \hat{Z}_1 \mid n\lambda\rangle$$
$$\mathcal{Z}_{2mn} = \langle m\lambda \mid \hat{Z}_2 \mid n\lambda\rangle$$
$$\mathcal{Z}_{3mn} = \langle m\lambda \mid \hat{Z}_3 \mid n\lambda\rangle$$

Example:

consider hamiltonians of the form:

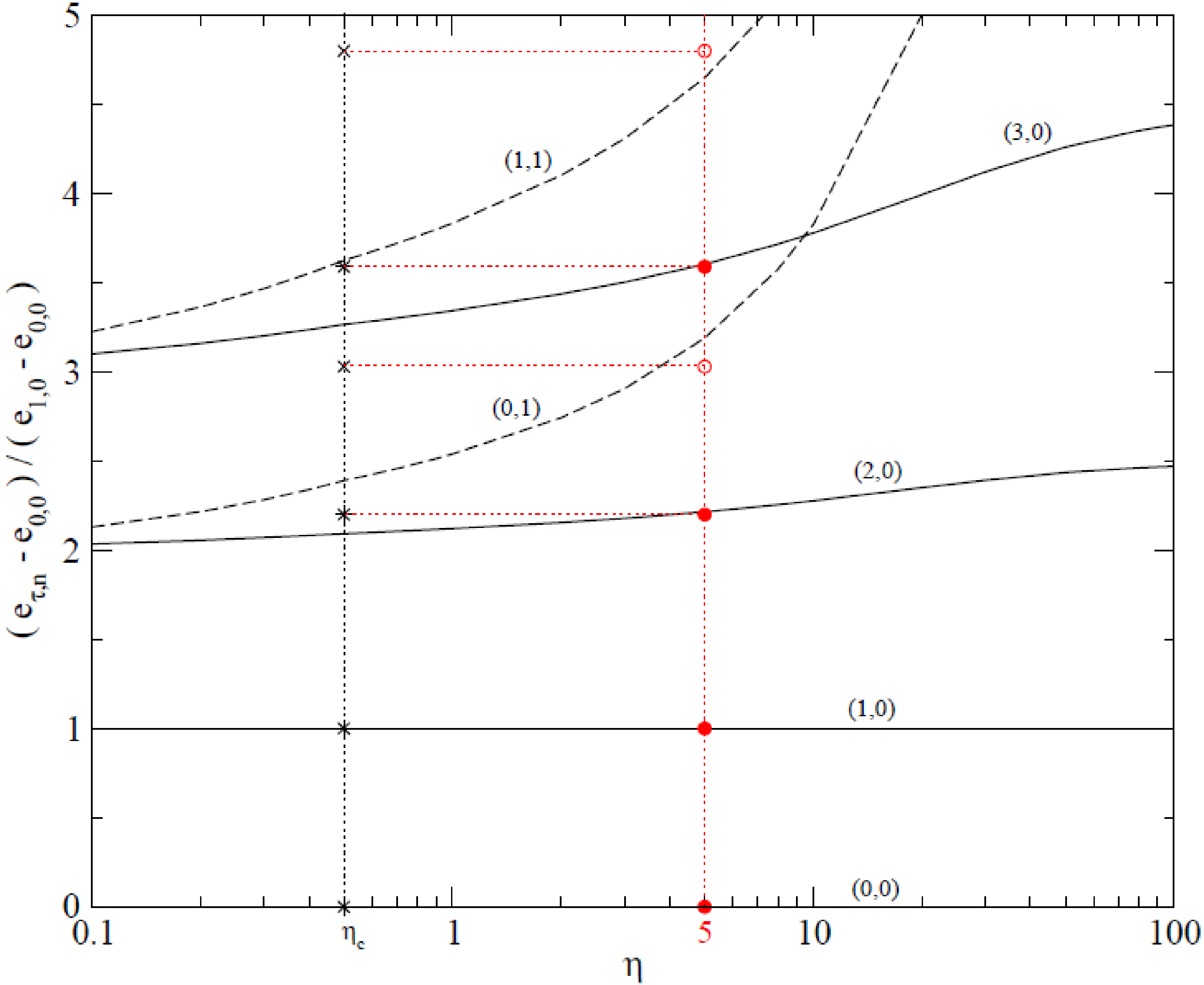
$$\hat{H} = \frac{1}{2}\mathrm{p}^2 + \alpha \mathrm{r}^{2M} = \frac{1}{2}\hat{Z}_1 + \alpha \hat{Z}_2^{2M}.$$

we take $M = 2$. Then $\hat{H} = \frac{1}{2}Z_1 + \alpha Z_2^2$ and

$$H_{mn} = \langle m\lambda \mid \hat{H} \mid n\lambda\rangle = \frac{1}{2}\langle m\lambda \mid \hat{Z}_1 \mid n\lambda\rangle + \alpha \sum_k \langle m\lambda \mid \hat{Z}_2 \mid k\lambda\rangle\langle k\lambda \mid \hat{Z}_2 \mid n\lambda\rangle$$

Then diagonalize the matrix (truncated at a certain n-max) and find the spectrum!

Example: van Roosmalen potential



From Camerino workshop 2005. Work inspired by Franco's E(5) solution and the thesis of one of his students (O. van Roosmalen).

$$u(\beta) = \frac{(1-\eta)}{2}\beta^2 + \frac{\eta}{4}(1-\beta^2)^2$$

Generalization to two coordinates

$$Z_1 = \mathbf{p}_1^2 \qquad Z_2 = \mathbf{r}_1^2 \qquad Z_3 = -\frac{i}{2}(\mathbf{p}_1 \cdot \mathbf{r}_1 + \mathbf{r}_1 \cdot \mathbf{p}_1)$$

$$Z_4 = \mathbf{p}_2^2 \qquad Z_5 = \mathbf{r}_2^2 \qquad Z_6 = -\frac{i}{2}(\mathbf{p}_2 \cdot \mathbf{r}_2 + \mathbf{r}_2 \cdot \mathbf{p}_2)$$

$\rightarrow sp(2) \oplus sp(2)$

$$Z_7 = \mathbf{p}_1 \cdot \mathbf{p}_2 \qquad Z_8 = \mathbf{r}_1 \cdot \mathbf{r}_2$$

$$Z_9 = i\mathbf{p}_1 \cdot \mathbf{r}_2 \qquad Z_{10} = i\mathbf{r}_1 \cdot \mathbf{p}_2$$

$\rightarrow sp(4)$

$$r_{12} = | \mathbf{r}_1 - \mathbf{r}_2 | = \sqrt{r_1^2 + r_2^2 - 2\mathbf{r}_1 \cdot \mathbf{r}_2}.$$

Interparticle distance !
This allows to introduce mutual interactions between particles!
Think to the possibilities!

They close into the sp(4) Lie algebra

	Z_1	Z_2	Z_3	Z_4	Z_5	Z_6	Z_7	Z_8	Z_9	Z_{10}
Z_1	0	$-4iZ_3$	$-2iZ_1$	0	0	0	0	$-2Z_9$	0	$2Z_7$
Z_2		0	$2iZ_2$	0	0	0	$2Z_{10}$	0	$-2Z_8$	0
Z_3			0	0	0	0	iZ_7	$-iZ_8$	iZ_9	$-iZ_{10}$
Z_4				0	$-4iZ_6$	$-2iZ_4$	0	$-2Z_{10}$	$2Z_7$	0
Z_5					0	$2iZ_5$	$2Z_9$	0	0	$-2Z_8$
Z_6						0	iZ_7	$-iZ_8$	$-iZ_9$	iZ_{10}
Z_7							0	$-iZ_3 - iZ_6$	Z_1	Z_4
Z_8								0	$-Z_5$	$-Z_2$
Z_9									0	$-iZ_3 + iZ_6$

Commutation relations $[row, col]$

Commutators of the type $[Z_{>i}, Z_i]$ are found by antisymmetry.

The structure constants and root system are those of the sp(4) ~ so(5) Lie algebra: this is checked also with the GAP computer program that allows for symbolic calculations.

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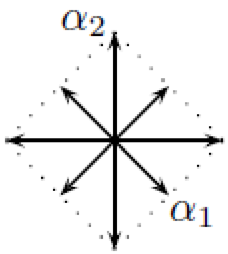
1° mapping to Cartan-Weyl form and root diagram

$$Z_1 = 2X_0 + X_+ + X_- \qquad Z_4 = 2Y_0 + Y_+ + Y_-$$
$$Z_2 = 2X_0 - X_+ - X_- \qquad Z_5 = 2Y_0 - Y_+ - Y_-$$
$$Z_3 = i(X_- - X_+) \qquad Z_6 = i(Y_- - Y_+)$$

$$Z_7 = \frac{1}{4}(-T_{--} + T_{-+} + T_{+-} + T_{++})$$
$$Z_8 = \frac{1}{4}(T_{--} + T_{-+} + T_{+-} - T_{++})$$

$$Z_9 = \frac{1}{4}(T_{--} + T_{-+} - T_{+-} + T_{++})$$
$$Z_{10} = \frac{1}{4}(T_{--} - T_{-+} + T_{+-} + T_{++})$$



$$\alpha_1 = [1,-1]_{FWS}$$
$$\alpha_2 = [0,2]_{FWS}$$
$$\alpha_3 = [1,1]_{FWS}$$
$$\alpha_4 = [2,0]_{FWS}$$

C_2 roots in the fundamental weight system FWS

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2° Mapping to bosonic operators

$$X_0 = \frac{1}{2}\left(b_2^\dagger b_2 - b_1^\dagger b_1\right) \qquad Y_0 = \frac{1}{2}\left(b_4^\dagger b_4 - b_3^\dagger b_3\right)$$

$$X_+ = -i b_2^\dagger b_1 \qquad Y_+ = -i b_4^\dagger b_3$$

$$X_- = -i b_1^\dagger b_2 \qquad Y_- = -i b_3^\dagger b_4$$

$$T_{--} = \frac{1}{2}\left(-b_4^\dagger b_1 - b_2^\dagger b_3\right) \qquad T_{++} = \frac{1}{2}\left(-b_1^\dagger b_4 - b_3^\dagger b_2\right)$$

$$T_{+-} = \frac{i}{2}\left(b_4^\dagger b_2 + b_1^\dagger b_3\right) \qquad T_{-+} = \frac{i}{2}\left(-b_2^\dagger b_4 - b_3^\dagger b_1\right)$$

4 bosonic modes

$$|\, a, b, c, d\rangle = N(a, b, c, d)\xi_1^a \xi_2^b \xi_3^c \xi_4^d$$

$$b_i = \partial/\partial \xi_i$$

$$b_i^\dagger = \xi_i$$

Monomials in the 4 variables

$$a \leftrightarrow n \qquad b \leftrightarrow -\lambda - n \qquad c \leftrightarrow m \qquad d \leftrightarrow -\mu - m$$

Obtained from the comparison of Casimir operators (there are dual relationships, but these are simpler)

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Action of the operators on the basis states

$$X_0 \mid n\lambda m\mu\rangle = (n+\lambda/2) \mid n\lambda m\mu\rangle$$
$$X_+ \mid n\lambda m\mu\rangle = \sqrt{(\lambda+n)(n+1)} \mid n+1, \lambda, m\mu\rangle$$
$$X_- \mid n\lambda m\mu\rangle = \sqrt{(\lambda+n-1)n} \mid n-1, \lambda m\mu\rangle$$

The corresponding action of the Y operators is obtained by replacing $\lambda \leftrightarrow \mu$ and $n \leftrightarrow m$.

$$T_{++} \mid n\lambda m\mu\rangle = -\frac{i}{2}\sqrt{(\mu+m)(n+1)} \mid n+1, \lambda-1, m, \mu+1\rangle + \frac{i}{2}\sqrt{(\lambda+n)(m+1)} \mid n, \lambda+1, m+1, \mu-1\rangle$$
$$T_{--} \mid n\lambda m\mu\rangle = -\frac{i}{2}\sqrt{(\mu+m-1)n} \mid n-1, \lambda+1, m, \mu-1\rangle + \frac{i}{2}\sqrt{(\lambda+n-1)m} \mid n, \lambda-1, m-1, \mu+1\rangle$$
$$T_{-+} \mid n\lambda m\mu\rangle = -\frac{i}{2}\sqrt{(\lambda+n-1)(\mu+m)} \mid n, \lambda-1, m, \mu+1\rangle - \frac{i}{2}\sqrt{n(m+1)} \mid n-1, \lambda+1, m+1, \mu-1\rangle$$
$$T_{+-} \mid n\lambda m\mu\rangle = \frac{i}{2}\sqrt{(\lambda+n)(\mu+m-1)} \mid n, \lambda+1, m, \mu-1\rangle + \frac{i}{2}\sqrt{(n+1)(m+1)} \mid n+1, \lambda-1, m-1, \mu+1\rangle$$

This is new !

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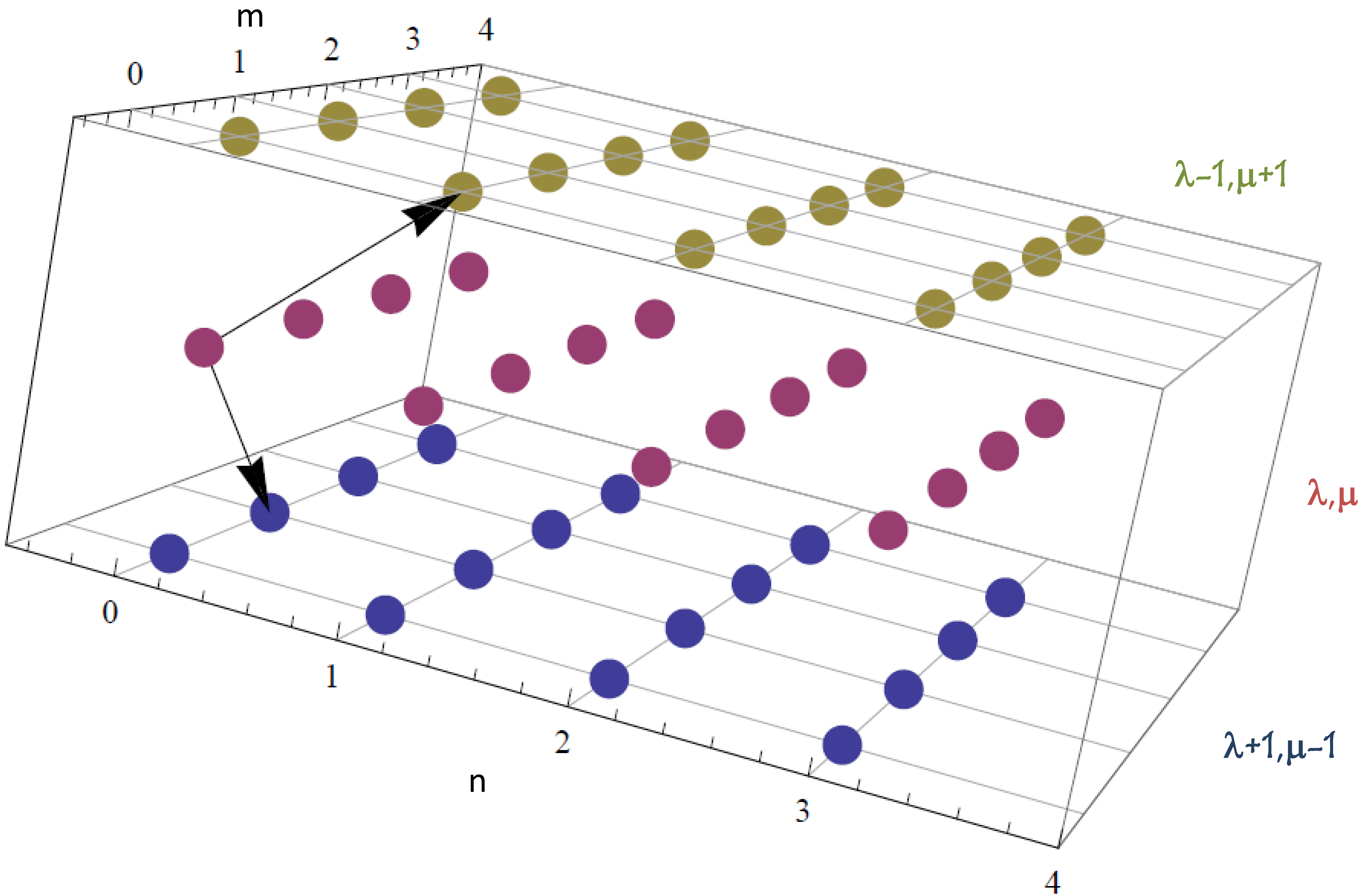
Action of T++



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Summary so far

p^2 and r^2 PHYSICS → Z-operators ALGEBRA → X-operators ROOT DIAGRAM → Bosonic oper. ACTION

$$Z_1 = \begin{pmatrix} \frac{3}{2} & 0 & \sqrt{\frac{3}{2}} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{3}{2} & 0 & 0 & 0 & 0 & 0 & 0 \\ \sqrt{\frac{3}{2}} & 0 & \frac{7}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{3}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{3}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{5}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{5}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{7}{2} \end{pmatrix}$$

$$Z_2 = \begin{pmatrix} \frac{3}{2} & 0 & -\sqrt{\frac{3}{2}} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{3}{2} & 0 & 0 & 0 & 0 & 0 & 0 \\ -\sqrt{\frac{3}{2}} & 0 & \frac{7}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{3}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{3}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{5}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{5}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{7}{2} \end{pmatrix}$$

This is how you set up hamiltonian-matrices

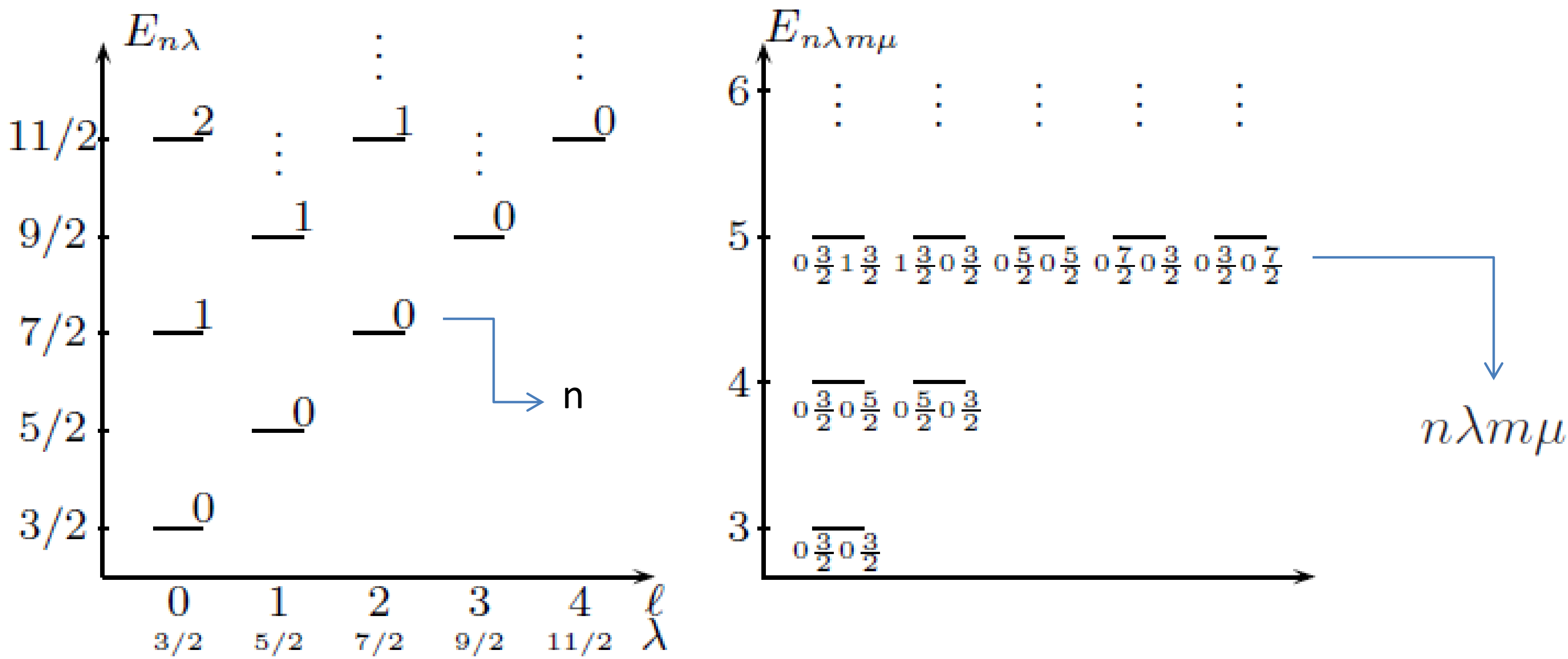
$$\begin{pmatrix} 3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 5 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 5 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 4 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 5 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 4 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 5 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 5 \end{pmatrix} = H = (Z_1 + Z_2 + Z_4 + Z_5)/2$$

$$H' = (Z_1 + Z_2 + Z_4 + Z_5 * Z_5)/2$$

$$\begin{pmatrix} \frac{33}{8} & -\sqrt{6} & 0 & 0 & 0 & 0 & 0 & 0 \\ -\sqrt{6} & \frac{81}{8} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{43}{8} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{47}{8} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{75}{8} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{35}{8} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{55}{8} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{43}{8} \end{pmatrix}$$

Trivial application: two indep. H.O.

$$H = (\mathbf{p}_1^2 + \mathbf{p}_2^2 + \mathbf{r}_1^2 + \mathbf{r}_2^2)/2 = (Z_1 + Z_2 + Z_4 + Z_5)/2$$



This probes only the sp(2)⊕sp(2) part of the algebra (it's a double copy of Rowe's)

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More challenging test of the sp(4) m.e.

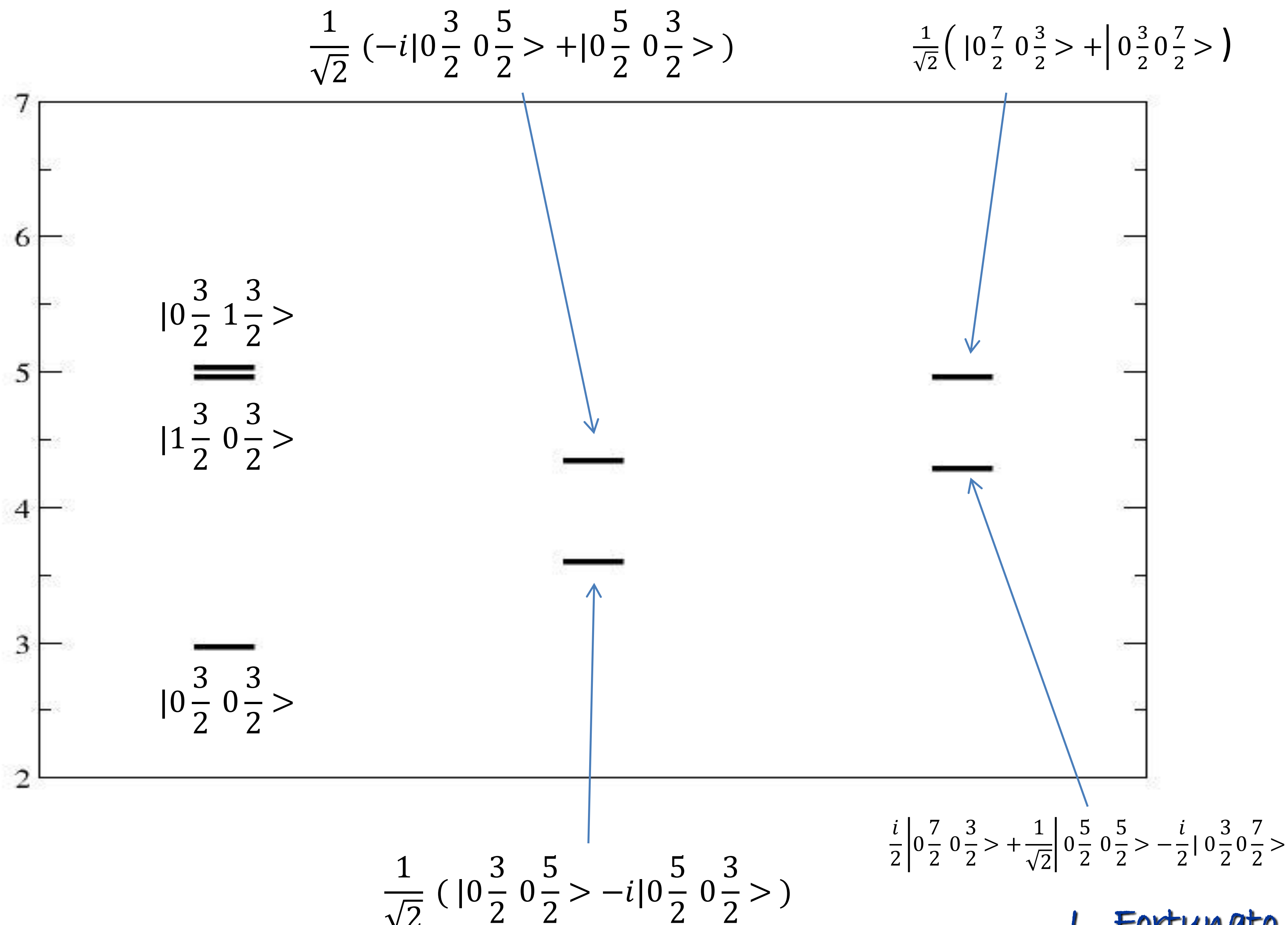
$$
\begin{aligned}
H &= (\mathbf{p}_1^2 + \mathbf{p}_2^2 - 2\mathbf{p}_1 \cdot \mathbf{p}_2 + \mathbf{r}_1^2 + \mathbf{r}_2^2 - 2\mathbf{r}_1 \cdot \mathbf{r}_2)/2 \\
&= \frac{1}{2}(\mathbf{p}_1 - \mathbf{p}_2)^2 + \frac{1}{2}(\mathbf{r}_1 - \mathbf{r}_2)^2 \\
&= (Z_1 + Z_2 - 2Z_7 + Z_4 + Z_5 - 2Z_8)/2
\end{aligned}
$$

This hamiltonian probes the genuine sp(4) part of the algebra. A subset of the spectrum must brew up to give a harmonic oscillator pattern:

Eigenvalues = { 13., 13., 13., 13., 13., 13., 13., 13., 13., 13., 13., 13., 13., 13., 13., 13., 13., 13., 13., 13., 13., 11., 11., 11., 11., 11., 11., 11., 11., 11., 11., 11., 11., 11., 11., 11., 9., 9., 9., 9., 9., 9., 9., 9., 9., 9., 7., 7., 7., 7., 7., 7., 5., 5., 5., 3.}

Matrices here are just 56 x 56 having used all the $\lambda=\mu=0$ states up to 10 quanta
One gets exact energies and exact degeneration patterns.

Lowest eigenstates



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A new 3D analytic solution!

$$H = \frac{\mathbf{p}_1^2}{2m} + \frac{\mathbf{p}_2^2}{2m} + k\frac{\mathbf{r}_1^2}{2} + k\frac{\mathbf{r}_2^2}{2} + k'\frac{r_{12}^2}{2}$$
$$= Z_1/2m + Z_4/2m + kZ_2/2 + kZ_5/2 + k' r_{12}^2/2$$

Now, please guess the energy of the ground state of this hamiltonian!
Take $\hbar$=k=k'=m=1 for simplicity.

Come on, time's ticking away!

$$E_{g.s.} = 3\sqrt{2}$$

A subset of the eigenstates has nice mathematical expressions.
Numerical solution gives: 4.24264, 7.07107, 9.89949, ...
that are nothing but : $3\sqrt{2}$, $5\sqrt{2}$, $7\sqrt{2}$, ...

I have now an analytic proof of this fact based on a 6D argument.
This is a generalization to 3D of known 1D models (Morse-Feshbach)

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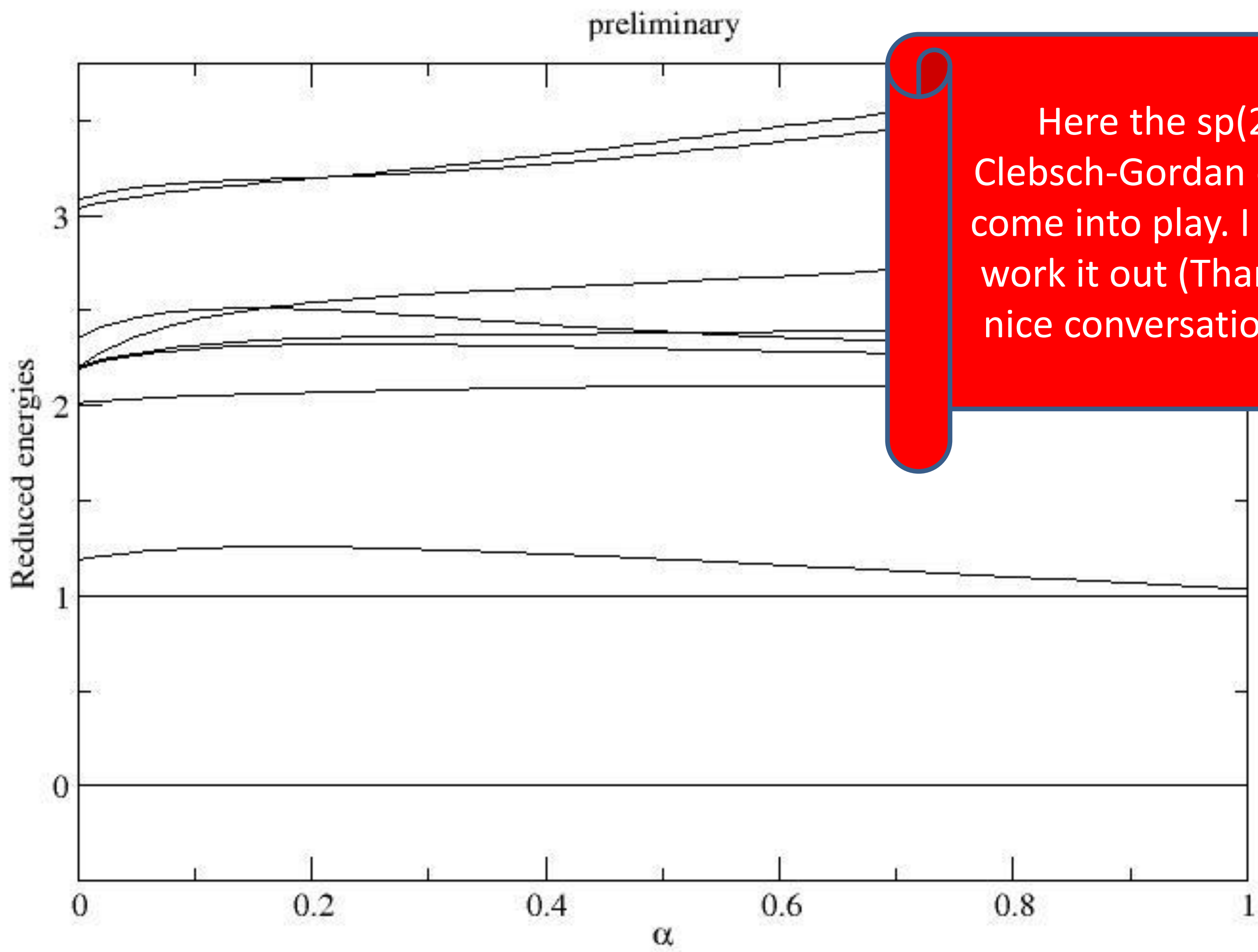
An interesting model for pairing interaction

Choose a Landau-type potential for the mutual interaction between particles

$$
\begin{aligned}
H &= (\mathrm{p}_1^2 + \mathrm{p}_2^2 + \mathrm{r}_1^2 + \mathrm{r}_2^2)/2 + \overbrace{\left(\frac{1}{2} - \alpha\right) r_{12}^2 + \alpha r_{12}^4}^{V(r_{12})} \\
&= (Z_1 + Z_2)/2 + \left(\frac{3}{2} - \alpha\right)(Z_2 + Z_5) + (\alpha - 1) Z_7 \; + \; \alpha (Z_2 + Z_5 - 2Z_7)^2
\end{aligned}
$$

- There is no reason why this should be a phase transition, $V(r_{12})$ is only part of the total potential felt by the two particles.
- Eigenstates will be mixtures of states with good quantum numbers $|n\lambda m\mu >$
- Do we need projection on states of good total angular momentum?
- Clebsch-Gordan coefficients for su(1,1)

Spectrum



Here the sp(2)+sp(2) Clebsch-Gordan coefficients come into play. I still have to work it out (Thanks Piet for nice conversation on this).

Perspective

Very general problems become tractable :

- Let's say 20 quanta
- Matrix element calculation time about 1 min
- Diagonalization of 'reasonable' hamiltonians in 5 seconds or so...

$$\mathrm{H} = \frac{p_1^2}{2m} + \frac{p_2^2}{2m} + V_A(r_1^2) + V_B(r_2^2) + V_C(r_{12}^2)$$

One could treat equally well operators with higher powers of p^2 or with velocity dependent terms (remember $\overrightarrow{r_i} \cdot \overrightarrow{p_j}$ are also elements of the algebra).

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Summary: a whole new approach

- A useful realization of the sp(4) Lie algebra has been introduced that contains important scalar operators made up with positions and momenta of two coordinates
- This algebra has been mapped to Cartan-Weyl form (to identify step and weight operators) and then mapped to Bosonic operators (to easily calculate matrix elements)
- A large class of three-body hamiltonians can be written as polynomials in the elements of sp(4) and then diagonalized in a properly truncated doubly-infinite basis
- [Do you have suggestions for important/useful applications? Atomic physics? Quantum dots? Molecular physics? Ab initio calculations?]

Extensions and developments are in sight:

1. 3D Calogero-Sutherland models (!)
2. Isomorphical S.G.A. for the **Helium atom – exact treatment** (!!!)
3. 3 coordinates very general **exact four-body problems** based on sp(6) (!!!)
4. etc. sp(2n)

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Thanks FRANCO for stirring the course of our field of studies with a firm hand into such a beatiful sea of symmetries in physics

and

thank you for your attention

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