

Algebraic approach to scattering

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Summary

- Motivation
- Algebraic description of the structure of bound systems.
- Algebraic description of the structure of unbound systems.
J. Phys. **A37**:Math.Gen. (2004) 1805-1820.
- Algebraic description of the scattering of systems with internal structure.
J. Phys. B: At. Mol. Opt. Phys. 40 (2007) 4513-4527.

Motivation: What is an algebraic approach?

- Associate the Hilbert space for a given system with the subspace that generates a certain irreducible representation of a group. This is the Dynamic group of the system.
- Choose a basis for the Hilbert space with labels of the group.
- Expand all relevant operators (including the hamiltonian) in terms of the generators of the group
- Obtain eigenstates diagonalizing the hamiltonian.
- Obtain transition matrix elements using the algebraic expressions of the matrix elements of the generators in the irrep basis.

Motivation: Why an algebraic approach?

- An algebraic model can extract the main features of a complex system, without the need of knowing in detail the interactions of the system, or solving equations in configuration space.
- An algebraic approach is useful if all relevant operators can be expanded in terms of low powers of the generators.

	Analytic	Algebraic
Wavefunctions	$\Psi(\xi_1, \xi_2, \dots)$	$ j_1 m_1, j_2 m_2 \dots \rangle$
Hamiltonian	$H = T + V$	$H = \sum_i c_i J_i + \dots$
Operators	$O = O(\xi_i)$	$O = \sum_i e_i J_i + \dots$
Eigenstates	Solve dif. eq.	Diagonalize H

Bound states: SU(2)

- Hilbert space: N vibrational bound states of a molecule.
- Dynamic group: SU(2)
- Generators: J^+, J^-, J_z
- Irreducible representation:
 $\{|jm\rangle, m = -j, j\}; 2j + 1 = N$
- Hamiltonian: $H = a + bJ_z + cJ^+ + c^*J^- + dJ_z^2 + \dots$

A particular realization: The Morse Potential

- States:

$$|jm\rangle \equiv \Psi_v^j(y) = N_v^j e^{-\frac{y}{2}} y^{j-v} L_v^{2(j-v)}(y),$$

$$v = j - m; y = Ce^{-\beta x},$$

- Hamiltonian

$$(1) \quad H = T + V \equiv -aJ_z^2$$

- Interaction

$$(2) \quad V(x) = D(e^{-2\beta x} - 2e^{-\beta x}),$$

Bound and unbound states: SU(1,1)

- Hilbert space: N vibrational bound states of a molecule plus the continuum of unbound states.
- Dynamic group: SU(1,1)
- Generators: K^+, K^-, K_0

$$[\hat{K}_+, \hat{K}_-] = -2\hat{K}_0, \quad [\hat{K}_0, \hat{K}_-] = -\hat{K}_-, \quad [\hat{K}_0, \hat{K}_+] = \hat{K}_+,$$

- Irreducible representation: $\{|\sigma m \rangle, m = \sigma, \sigma + 1, \dots\}$

$$\hat{K}_+ |\sigma, m \rangle = \sqrt{(m + \sigma)(m - \sigma + 1)} |\sigma, m + 1 \rangle,$$

$$\hat{K}_- |\sigma, m \rangle = \sqrt{(m - \sigma)(m + \sigma - 1)} |\sigma, m - 1 \rangle,$$

$$\hat{K}_0 |\sigma, m \rangle = m |\sigma, m \rangle,$$

- Hamiltonian: $H = a + bK_0 + cK_+ + c^*K_- + \dots$

A particular realization: The Morse Potential

- States:

$$|\sigma m\rangle \equiv \Phi_n^\sigma(y) = A_n^\sigma L_n^{2\sigma-1}(y) y^\sigma e^{-y/2}, \quad n = 0, 1, 2, \dots$$

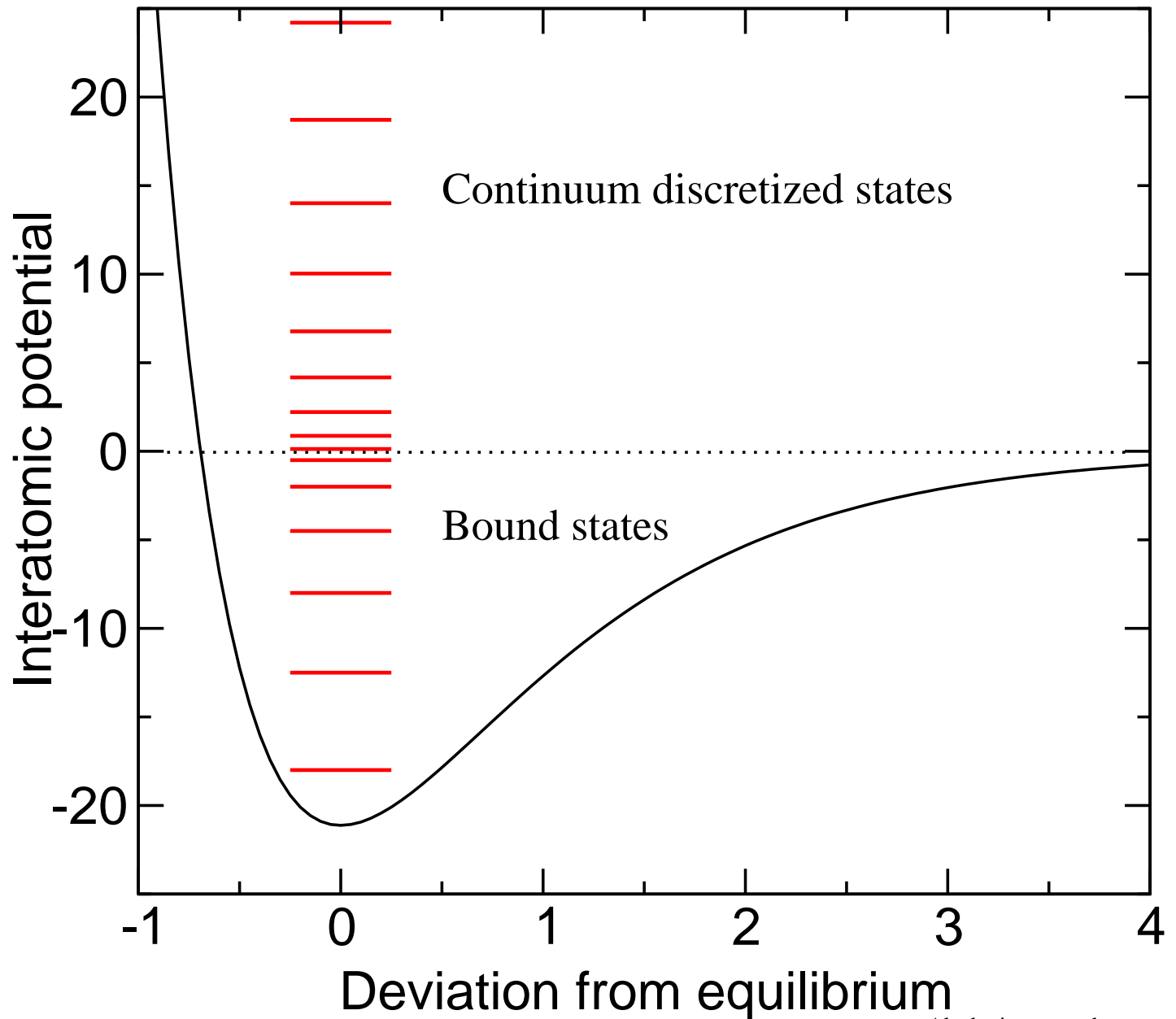
$$m = \sigma + n; \quad y = (2j + 1)e^{-\beta x},$$

- Hamiltonian

$$\begin{aligned} \hat{H} &= \frac{\hbar^2 \beta^2}{2\mu} \left\{ -\sigma(\sigma - 1) \right. \\ &\quad + \hat{K}_0(2\hat{K}_0 - 2j - 1) + (j + 1/2)(\hat{K}_+ + \hat{K}_-) \\ &\quad \left. - \frac{1}{2}[(\hat{K}_+ + \hat{K}_-)\hat{K}_0 + \hat{K}_0(\hat{K}_+ + \hat{K}_-)] \right\}, \end{aligned}$$

- Basis: Diagonalize H in an $SU(1,1)$ basis of N states.
- Choosing $\sigma = j$, bound states decouple from the continuum states.

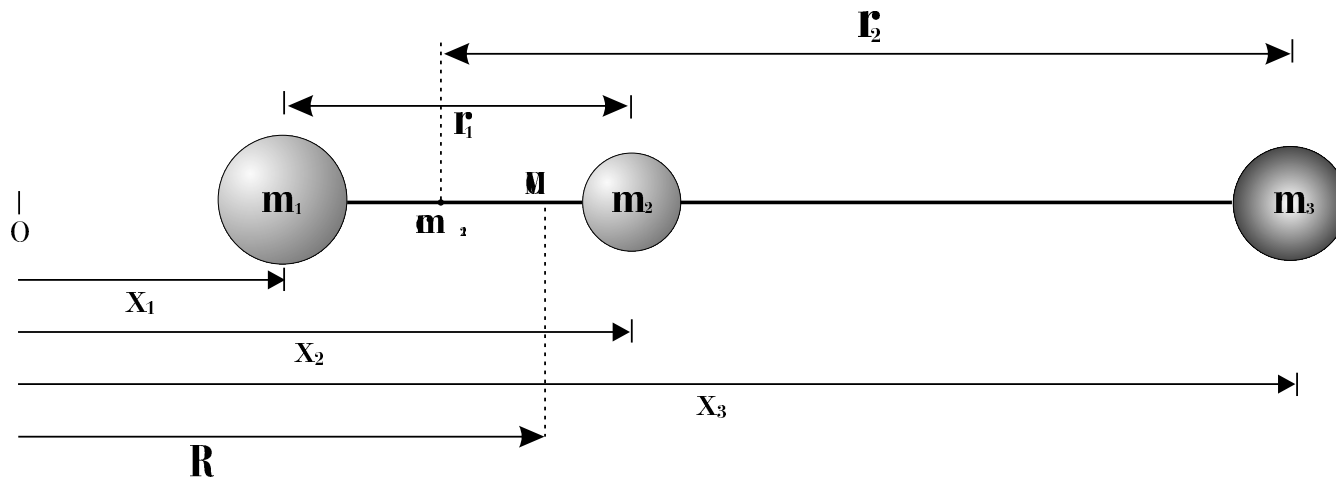
Diatomic molecules



Dipole matrix elements

N	$n=0$		$n=3$	
	$S(\hat{\mu}, N)$	$E_W(\hat{\mu}, N)$	$S(\hat{\mu}, N)$	$E_W(\hat{\mu}, N)$
6	0.0181201	0.203022	0.0461536	0.397858
8	0.0181261	0.202675	0.0485419	0.342468
10		0.202672	0.0487340	0.338792
20			0.0487918	0.337513
30			0.0487931	0.337464
Exact Value	0.0181261	0.202672	0.0487933	0.337450

Molecular collisions



- Total Hamiltonian

$$\hat{\mathcal{H}} = \hat{H}_M - \frac{1}{2m} \frac{\partial^2}{\partial x^2} + V_{AB}(x - y),$$

- Internal Hamiltonian

$$\hat{\mathcal{H}}_I = \hat{\mathcal{H}} - \mathcal{H}_{cl} = \hat{H}_M(p, y) + \hat{V}(y, t),$$

Evolution operator

$$(3) \quad |\psi(t)\rangle = U_0(t, t_0)U_I(t, t_0)|\psi_M(t_0)\rangle,$$

Where $U_0(t, t_0) = e^{-i\hat{H}_M(t-t_0)}$. The evolution operator $U_I(t)$ satisfies

$$(4) \quad i\frac{d}{dt}U_I(t) = \hat{V}_I(t)U_I(t),$$

where

$$(5) \quad \hat{V}_I(t) = U_0^\dagger(t)\hat{V}(t)U_0(t).$$

Algebraic approximation

$$(6) \quad \hat{V}_I(t) \simeq \sum_i \alpha_i(t) \hat{X}_i.$$

$$(7) \quad U_I(t) = \prod_i \exp[-ig_i(t) \hat{X}_i],$$

$$(8) \quad \hat{S} = U_I(\infty, -\infty) = \prod_i \exp[-ig_i(\infty) \hat{X}_i],$$

The S-matrix is a representation of a certain element of the group

Application to excitation to bound states: SU(2)

$$(9) \quad \hat{V}_I(t) \approx \alpha_0(t) \hat{I} + \alpha_1(t) \hat{J}_x + \alpha_2(t) \hat{J}_y + \alpha_3(t) \hat{J}_z,$$

$$(10) \quad U_I(t) = e^{-ia_0(t)\hat{I}} e^{-ia_x(t)\hat{J}_x} e^{-ia_y(t)\hat{J}_y} e^{-ia_z(t)\hat{J}_z}.$$

$$\begin{pmatrix} \dot{\alpha}_0(t) \\ \dot{\alpha}_x(t) \\ \dot{\alpha}_y(t) \\ \dot{\alpha}_z(t) \end{pmatrix} = \mathbf{M}(t) \begin{pmatrix} \alpha_0(t) \\ \alpha_1(t) \\ \alpha_2(t) \\ \alpha_3(t) \end{pmatrix},$$

$$M(t) =$$

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & \sin(a_x(t)) \tan(a_y(t)) & -\cos(a_x(t)) \tan(a_y(t)) \\ 0 & 0 & \cos(a_x(t)) & \sin(a_x(t)) \\ 0 & 0 & -\sin(a_x(t)) / \cos(a_y(t)) & \cos(a_x(t)) / \cos(a_y(t)) \end{pmatrix}.$$

$$\hat{S} = U_I(\infty, -\infty) = e^{-ia_0\hat{I}} e^{-ia_x\hat{J}_x} e^{-ia_y\hat{J}_y} e^{-ia_z\hat{J}_z}.$$

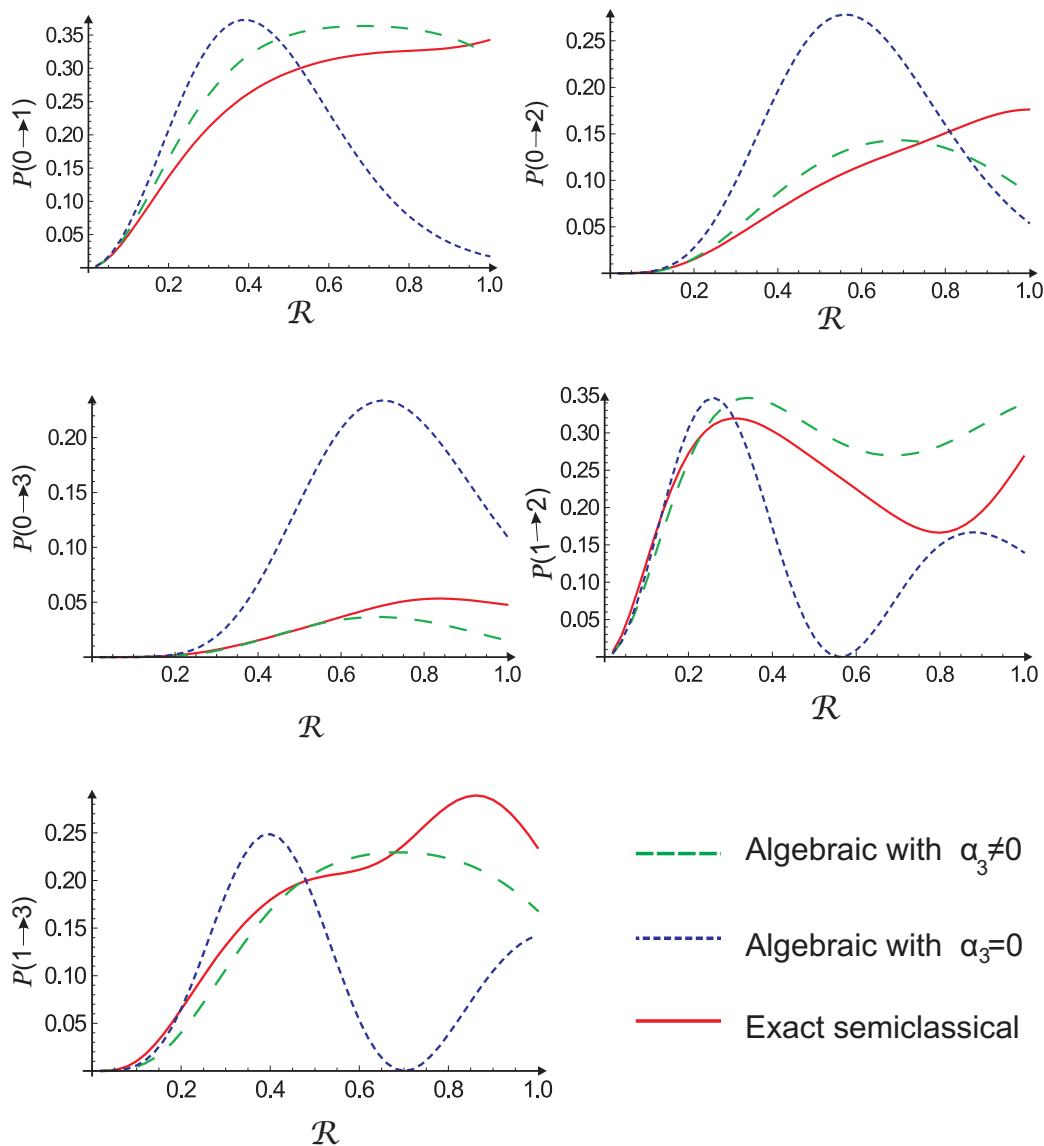
$$\langle jm|\hat{S}|jm'\rangle = \mathcal{D}_{m,m'}^j(\alpha, \beta, \gamma)$$

$$P_{n\rightarrow n'} = |d_{(j-n),(j-n')}^j(\beta)|^2$$

**Scattering on a vibrational molecule is
equivalent to a “Rotation”**

Comparison with semiclassical calculations

E=8



Comparison with quantum mechanical calculations

System: $H_2 + He$. $E=8 \hbar\omega$.

Quantum mechanical calculations: A P Clark and A S Dickinson
1973 J.Phys. B:Atom.Molec.Phys. **6** 164-180.

Parameter fitted: $\beta = 0.1960$

$P_{i \rightarrow f}$	$0 \rightarrow 1$	$1 \rightarrow 2$	$0 \rightarrow 2$	$0 \rightarrow 3$	$1 \rightarrow 3$	$2 \rightarrow 3$
C&D	2.45(-1)	3.18(-1)	3.38(-2)	2.72(-3)	5.72(-2)	3.34(-1)
Algebraic	2.46(-1)	3.06(-1)	3.41(-2)	2.33(-4)	5.22(-2)	3.15(-1)

Outlook

- Obtain the S-matrix for $SU(1,1)$, and describe dissociation of molecules. (Short term).
- Use continuum representations of $SU(1,1)$ and other non-compact groups to describe the continuum. (???)
- Use non-compact groups to describe weakly bound nuclei ($U(3,1)$?)
- Relate CDCC S-matrices with the representation of some group (Long term wish)