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Lie Algebraic Approaches to Advanced Few-Body Hamiltonians in Physics

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Abstract In quantum many-body systems, the emergence of complex interactions generally prevents the straightforward application of conventional analytical methods such as direct solution of the Schrödinger equation, variation theory, or the WKB approximation. An alternative algebraic perspective, employing techniques such as representation theory, reduction transformations, and gauge transformations, provide successful ways by identifying the hidden Lie algebra underlying a given problem.

On the other hand, few-body systems remain challenging, as their symmetries are limited rather than N-body cases. In this work, we demonstrate that by incorporating geometric insight, one may establishes a meaningful connection between the mathematical structure and the physical content of the problem.

Keywords. Lie algebraic approach, geometry, two-body and three-body problem, Hellmann potential

1 Introduction

Since the early twentieth century and the development of quantum mechanics, it became clear that new mathematical frameworks were required. The use of Lie algebra representations in solving problems such as the simple harmonic oscillator and the hydrogen atom constituted early successful efforts in this direction [1]. Beginning around 1970, mathematical physicists such as Calogero, Perelomov, and others systematically applied Lie algebraic methods to the study of quantum N-body systems [2, 3]. In such systems, symmetry simplifies many relations and often leads to closed-form expressions for wave functions and eigenvalues.

Group theory allows classification of the possible quantum states of a system purely on the basis of its symmetries (e.g., rotational, translational, and permutation symmetry), and even enables prediction of system behavior prior to explicitly solving the Schrödinger equation or experiencing the true results in the lab. A familiar example is the hydrogen atom. Its symmetry is described by the group $SO(4)$, which extends beyond the ordinary spherical symmetry $SO(3)$ [4]. The Radial part of the Hydrogen atom in terms of Schrodinger equation simplifies to

$$-\frac{1}{\rho^2}\frac{d}{d\rho}(\rho^2\frac{dR(\rho)}{d\rho})+[-\frac{l(l+1)}{\rho^2}+\frac{2}{\rho}-\varepsilon]R(\rho)=0 \qquad (1)$$

Moreover, using the rotational symmetry and invariance of the Runge–Lenz vector in the hydrogen atom,

$$M^2=\frac{1}{4}(-1-\frac{\mu}{2H(n,l)}) \qquad (2)$$

One can directly obtain the energy eigenvalues by acting on the wave function

$$\varepsilon=-\frac{\mu}{2n^2} \qquad (3)$$

However, in few-body systems, the structure of the systems have limited geometrical symmetries respect to the N-body cases. In fact, infinite representations of the symmetry in the systems in few-body problems, changes to the specified geometric structures governing the system [5, 6]. By introducing a geometric perspective, one can take an effective step toward solving the problem. In this work, we employ this geometric interpretation to analyze two few-body physical problems and obtain their energy spectra.

2 From Differential Equations to Hidden Algebraic Structure: A Historical Perspective

A manifest symmetry is a transformation readily visible in the geometry of the system, such as the rotational symmetric

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operators in a sphere. A hidden symmetry, by contrast, is not apparent in configuration space but is encoded in the governing equations (e.g., the Schrödinger equation) and profoundly controls physical properties such as the energy spectrum.

The identification of hidden symmetry proceeds through the following steps:

1. For a given Hamiltonian H, identify a set of operators O_i: $[H, O_i] = 0$
2. Verify closure of the algebra generated by these operators $[O_i, O_j] = \imath\hbar f_{ij}^{k} O_k$
3. Compare the resulting algebraic relations with known Lie algebras $gl(n,R)$, $sl(n,R)$, $so(n)$, $su(n)$, … to reveal the underlying algebra of the problem.

Following the introduction of quantum N-body models by Calogero and Sutherland, these systems became a fertile area of research in both mathematics and physics [7]. In these models, particles are arranged on a symmetric lattice and interact through inverse-square rational or trigonometric potentials

$$
\begin{aligned}
H_{Cal} &= \frac{1}{2}\sum_{i=1}^{N}\left(-\frac{d^2}{dx_i^2} + \omega^2 x_i^2\right) + g\sum_{1\leq i<j\leq N}^{N}\frac{1}{(x_i - x_j)^2} \\
H_{Sut} &= \frac{1}{2}\sum_{i=1}^{N} -\frac{d^2}{dx_i^2} + g\sum_{1\leq i<j\leq N}^{N}\frac{1}{\sin^2(x_i - x_j)}
\end{aligned}
\tag{4}
$$

Calogero introduced Dunkl operators

$$
D_i = \frac{\partial}{\partial x_i} + \beta\sum_{i\neq j}^{N}\frac{1}{x_i - x_j}(1 - K_{ij}) \tag{5}
$$

and demonstrated that their commutation relations provide a sufficient condition for integrability and solvability

$$
[D_i, D_j] = 0 \tag{6}
$$

One of the pioneering algebraic approaches to the Calogero and Sutherland models was developed by Olshanetsky and Perelomov [8]. In this framework, the Hamiltonian is formulated in terms of the root system of a semi simple Lie algebra as a differential equation

$$
H = \frac{1}{2}\sum_{i=1}^{N} P_i^2 + \sum_{\alpha\in\phi^+}\frac{g}{(\alpha.x)^2}, \quad g = \beta(\beta - 1) \tag{7}
$$

For example, the rational Calogero model corresponds to a_n Lie algebra root system

$$
\phi^+ = e_i - e_j, \quad i < j \tag{8}
$$

While the Sutherland Hamiltonian represents its trigonometric version. The wave function is likewise determined by the root structure too:

$$
\psi_0(x) = \prod_{\alpha\in\phi^+}(\alpha.x)^2 \tag{9}
$$

In this sense, the hidden algebra of both models is the same, and the two potentials represent two aspects of a single algebraic structure. The essential idea is to relate symmetric spaces to quantum systems through representation theory, such that the Hamiltonian assumes the form of a Laplace Beltrami operator on the associated symmetric space.

In Turbiner's approach, one starts from the Hamiltonian derived from the root system and selects a polynomial space invariant under the Hamiltonian. For the Calogero Hamiltonian, such a space can be constructed explicitly

$$
a_n : V_n = \{x, x^2, x^3, \ldots, x^n\} \tag{10}
$$

One then identifies differential operators that act as generators of a Lie algebra (e.g., gl_n or sl_n) preserving this space by the algebraic generators

$$
\begin{aligned}
&J_i^- = \frac{\partial}{\partial x_i}, \quad J_{i,j}^0 = x_i J_j^-, \\
&J_0 = n - \sum_{i=1}^{N} x_p \frac{\partial}{\partial x_p}, \quad J_i^+ = x_i J_0
\end{aligned}
\tag{11}
$$

The Hamiltonian can then be rewritten as a second-degree polynomial in these generators and solved accordingly. In such systems, solvability arises from the existence of a hidden algebraic structure revealed through reduction [9].

Kamran's method begins from a fully mathematical standpoint, constructing the most general differential equation L_i based on first-order Lie algebra generators. By identifying an appropriate mapping, one establishes equivalence between the general quasi-exactly solvable operator

$$
T = \sum_{i,j=1}^{N} C_{ij} L_i L_j + \sum_{i=1}^{N} C_i L_i + C_0 \tag{12}
$$

and the Schrödinger equation. A central theorem in this case states that if a second-order differential operator satisfies certain structural conditions, based on Bochner's theorem, then through a suitable change of variables and gauge transformations, it can be cast into Schrödinger form with a well-defined potential [10, 11].

3 Few-Body Systems and Two Applications of the Algebraic–Geometric Approach

Many-body systems in nature are composed of interacting few-body subsystems. To understand thermodynamic, optical, and chemical properties of composite materials, one often first precisely characterize the quantum properties of their few-body building blocks. Quantum phenomena such as entanglement are more transparently observable in few-body systems. Although these effects persist in many-body systems, collective interactions complicate their control and

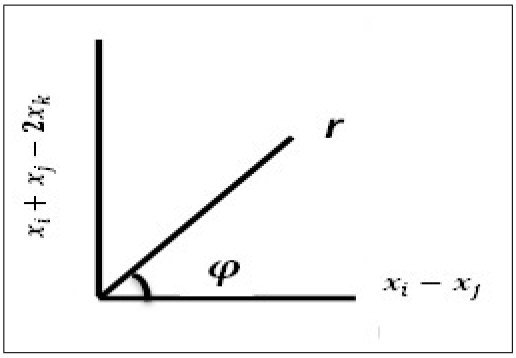

Fig. 1 Jacobi coordinates

analysis. Moreover, the development of quantum technologies such as quantum computing requires a detailed understanding of few-body systems [12].

For example, the exact solution of the Calogero Hamiltonian is expressed in terms of Jack polynomials

$$J_\lambda^\alpha(x_1, x_2, \ldots, x_N) = \sum_{\mu \le \lambda} c_{\mu\lambda}(\alpha) m_\mu(x_1, x_2, \ldots, x_N)$$
$$m_\mu(x_1, x_2, \ldots, x_N) = \sum x_1^{\lambda_1} x_2^{\lambda_2} \ldots x_N^{\lambda_N} \tag{13}$$

These polynomials are constructed from monomials m_μ corresponding to partitions of the system $\lambda = (\lambda_1, \lambda_2, \ldots, \lambda_N)$ by the condition $\lambda_1 \ge \lambda_2 \ge \ldots \ge \lambda_N$. For large particle numbers, writing these polynomials explicitly becomes highly nontrivial [13].

Another challenge arises in atoms with some valence electrons. Accounting for their interaction with lower-energy orbitals typically requires extensive computations not easily handled by conventional methods. We now examine two few-body problems within this algebraic–geometric framework.

3.1 A Three-Body Problem with Sutherland-Type Potential

Firstly, we consider a system of three distinguishable fermions interacting through two-body and three-body Sutherland-type potentials as follows [14]

$$H = \frac{1}{2}\sum_{i=1}^{3} -\frac{d^2}{dx_i^2} + g_\nu \sum_{1 \le i \ne j \le 3} \frac{1}{\sin^2(x_i - x_j)}$$
$$+ g_\mu \sum_{1 \le i \ne j \ne k \le 3} \frac{1}{\sin^2(x_i + x_j - 2x_k)} \tag{14}$$

By introducing Jacobi coordinates, Fig.1, the center-of-mass motion is separated from relative motion, revealing translational symmetry and reducing the number of variables

$$x_i - x_j = r\cos\phi, \quad x_i + x_j - 2x_k = r\sin\phi \tag{15}$$

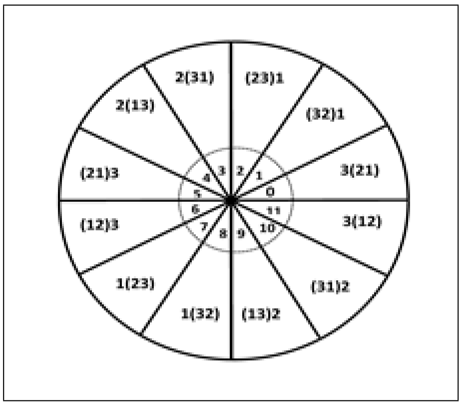

Fig. 2 D_{12} Lie group

The equation of motion separates into radial and angular parts

$$\left(-\frac{\partial^2}{\partial r^2} - \frac{1}{r}\frac{\partial}{\partial r} + \frac{\lambda^2}{r^2} - E\right)R(r) = 0$$
$$\left(-\frac{\partial^2}{\partial \phi^2} + \frac{9g_\nu}{\sin^2 3\phi} + \frac{9g_\mu}{\cos^2 3\phi} - \lambda^2\right)\Phi(\phi) = 0 \tag{16}$$

Consistency of the angular equation imposes a condition $\cos 6\phi \ne \pm 1$ leading to twelve admissible angular states, producing an elegant discrete symmetry in the problem. Due to the discrete symmetry associated with the Lie algebra D_{12}, Fig.2, in the reduced geometric space, the quantum calculations simplify considerably. Solving the Schrödinger equation in only one region of twelve configuration spaces suffices to determine all physical properties. Performing a reduction transformation and appropriate change of variables $z_j = \exp(2\imath a(R - x_{kl}))$, where $x_{kl} = x_k - x_l$ and $R = \frac{x_1 + x_2 + x_3}{3}$ the Hamiltonian separates into a center-of-mass term and a differential operator corresponding to a three-variable Jack polynomial structure

$$\tilde{H} = 6\frac{\hbar^2 a^2}{m}\left[\sum_{j=1}^{3}\left(z_j \frac{\partial}{\partial z_j}\right)^2 + (\nu + \mu) \sum_{j.k=1, j \ne k}^{3} \frac{z_j + z_k}{z_j - z_k}\left(z_j \frac{\partial}{\partial z_j}\right)\right]$$
$$+ \frac{4}{3}\frac{\hbar^2 a^2}{m}\left(\sum_{j=1}^{3} z_j \frac{\partial}{\partial z_j}\right)^2 \tag{17}$$

The resulting energy spectrum for the three distinguishable fermions is obtained in closed form

$$E_{rel} - E_0 = 4(\nu^2 - 3\mu^2 + 6(\nu + \mu) + 3) \tag{18}$$

3.2 B Screening in Alkali Atoms and the Hellmann Potential

Perturbation theory plays a central role in quantum mechanics; we apply Lie algebraic symmetry methods derived from

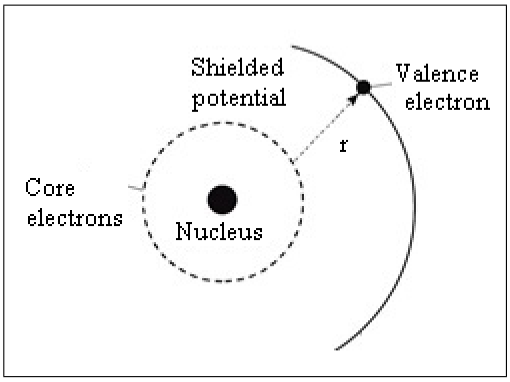

Fig. 3 Screening effect

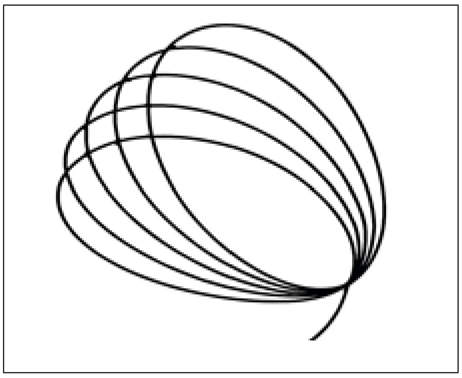

Fig. 4 Precession motion in the Hellmann potential

the hydrogen atom to the Hellmann potential, which is of Yukawa type added to Coulomb potential [15]

$$V(r) = -\frac{1}{r} + \frac{-Z}{r}\Upsilon e^{-\frac{\delta r}{Z}}, \quad \Upsilon = \frac{Z-1}{Z} \tag{19}$$

This potential arises naturally in alkali atoms, where inner electrons screen the nuclear charge experienced by the outermost electron, leading to deviations from the Coulomb potential and affecting the energy levels, Fig.3. The method proceeds by relating the perturbative term to the precessional motion of the Runge–Lenz vector

$$\overrightarrow{M} = \frac{1}{2\mu}(\overrightarrow{P} \times \overrightarrow{L} - \overrightarrow{L} \times \overrightarrow{P}) - \frac{Z}{r^2}\overrightarrow{r} \tag{20}$$

Whose Lie algebra $SO(4)$ is

$$so(4) = so(3) \bigoplus so(3) \tag{21}$$

And its Lie algebraic commutation relations are

$$\begin{aligned} &[L_i, L_j] = \imath\varepsilon_{ijk}L_k, \quad [L_i, M_j] = \imath\varepsilon_{ijk}M_k, \\ &[M_i, M_j] = \imath\varepsilon_{ijk}(-2\frac{E(n,l)}{\mu})L_k \end{aligned} \tag{22}$$

In the Hellmann potential, the Runge–Lenz vector undergoes precession, and the orbital ellipse is no longer closed, Fig.4. The perturbation effectively renders the algebra non-connected, which underlies the non-solvability of the system.

The perturbation could be corresponded as the Yukawa component of the Hellmann potential

$$p(r) = -\frac{Z-1}{r}\Upsilon)e^{-\frac{\delta r}{Z}} \tag{23}$$

The operator describing precession over one period T is

$$\Omega = \frac{\partial}{\partial L}(\frac{1}{T}\int p(r)dt) \tag{24}$$

We demonstrate that within the convergence domain determined by Cauchy estimates, stable energy eigenvalues can be obtained

$$|\frac{e^{-\frac{\delta r}{Z}}}{r}|_{R-\delta} \leq |\frac{-Z}{\delta r^2}|_R \tag{25}$$

Applying Kolmogorov's theorem [16]

$$p(r) \to O(-{\frac{Z}{\delta r^2}}^{2}) \tag{26}$$

Rewriting the Runge–Lenz vector operator within this approximation yields the corrected Hellmann potential spectrum.
Comparison with alternative computational methods shows good agreement for low-lying energy levels, Table 1, although discrepancies increase for higher levels due to more intricate interactions.

4 Conclusion and Discussion

Since 1969, significant progress has been made in solving many-body problems using Lie algebraic techniques. However, some of these methods are not fully effective for few-body systems. For example, specified symmetries exists for constructing wave functions of three- or four-body systems from the general N-body formalism, having more access to general symmetries and bigger geometric viewpoint.
From a practical standpoint, atoms with a finite number of interacting electrons present complex challenges in determining wave functions and energy spectra. In this work, by solving two such problems, we have shown that incorporating a geometric interpretation not only clarifies the physical meaning but also simplifies the solution procedure.
Nonetheless, this method has some limitations. Real physical systems frequently involve external fields, thermal effects, and explicit symmetry breaking. This demand could be answered

Table 1 comparison of our results and other methods

state	δ	our results	NU [17]	Ref [18]
$2P$	0.01	-0.07396007816	-0.077500	-0.072020
$3P$	0.01	-0.03297991942	-0.029279	-0.036644
$3d$	0.01	-0.04226536099	-0.043825	-0.036813
$4P$	0.01	-0.02561419824	-0.030925	-0.023641
$4d$	0.01	-0.04061691390	-0.031356	-0.023841
$4f$	0.01	-0.01894820393	-0.032356	-0.024056

1. The role of Lie algebra and group theory is to provide a precise structural understanding of the mathematical symmetries, while the ultimate solution of the physical problem depends on the specific dynamics;
2. According to Noether's theorem, symmetries are directly associated with conserved quantities. By first analyzing the ideal symmetric system and identifying its conserved quantities, one can then systematically investigate the geometric or algebraic mechanisms that break these symmetries. Thereby a more comprehensive understanding than a purely phenomenological approach would be provided.

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