Contact Symmetry of Time-Dependent Schrödinger Equation for a Two-Particle System: Symmetry Classification of Two-Body Central Potentials

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Abstract

Symmetry classification of two-body central potentials in a two-particle Schrödinger equation in terms of contact transformations of the equation has been investigated. Explicit calculation has shown that they are of the same four different classes as for the point transformations. Thus in this problem contact transformations are not essentially different from point transformations. We have also obtained the detailed algebraic structures of the corresponding Lie algebras and the functional bases of invariants for the transformation groups in all the four classes.

1 Introduction

The position of contact transformations [1, 2, 3, 4] lies in between the point transformations and the Lie-Bäcklund transformations [2, 5]. However, in studying the dynamics of a system the group of contact transformations has a very important position. Because of the continuity conditions in quantum mechanics of the wavefunction and its space derivatives, groups of contact transformations play such important roles in the dynamics of physical systems.

Point transformation groups for any set of differential equations involve transformations among the independent space-time variables and the dependent variables. The generators of the transformation group thus involve only these variables. The groups of contact transformations, on the other hand, involve these variables as well as the gradients of the dependent variables. The contact relations connecting the gradients with the original variables are thus included in the set of differential equations. If the generators do not involve the gradients in an essential manner, then the contact transformation group is not essentially different from the point transformation group [4].

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In a previous work [6] we have studied symmetry classification of two-body central potentials for the point transformation groups of time-dependent Schrödinger equation for a two-body system. Here, we have done a similar study of the groups of contact transformations of the same system. What we have found here, and what could not be known without this detailed analysis, is that the groups of contact transformations for this system are not essentially different from the corresponding groups of point transformations. Thus we have four classes of two-body central potentials:

1. a constant potential with a 31-parameter Lie group,
2. a harmonic oscillator potential with a 20-parameter Lie group,
3. an inverse square potential with a 16-parameter Lie group, and
4. all other potentials with a 14-parameter Lie group.

Using Lie-Jacobi’s method [4, 5] we have calculated the functional bases of invariants for all these cases. Any invariant of these groups can be functionally expressed in terms of these base invariants. For the constant potential case there are 5 base invariants. The corresponding number for all the other cases is 4.

2 Contact transformations and Schrödinger equation

The method [3] for obtaining the group of contact transformation is a generalization of the method of extended group [1, 2] for obtaining that of point transformations. We give below the essential points as it appears in our system of 2 particles of masses $m_1$ and $m_2$ at positions $\vec{r}_1$ and $\vec{r}_2$.

We use the relative space coordinate $\vec{r} = \vec{r}_1 - \vec{r}_2$, the centre-of-mass space coordinate $\vec{R} = (m_1\vec{r}_1 + m_2\vec{r}_2)/(m_1 + m_2)$, the reduced mass $m = m_1 m_2/(m_1 + m_2)$ and the total mass $M = m_1 + m_2$. It is to be noted that $0 < m/M \leq 1/4$. The limit $m/M = 1/4$ occurs when the two particles have equal masses. Positronium atom and a homonuclear diatomic molecule are two important physical systems which have this limiting value of $m/M$. The other limiting value $m/M = 0$ occurs when one of the masses and hence $M$ is $\infty$. This is same as ignoring the motion of the centre-of-mass. This does not describe a true two-body system and cannot thus throw any light on the classification of inter-particle potentials.

In terms of these variables, the 2-particle Schrödinger equation for the wavefunction $\Psi^0$ becomes

$$\Delta^0 \equiv i\Psi^0_{q^0} + \frac{\hbar}{2M} \sum_{\alpha} \Psi^{c\alpha}_{q^{c\alpha}} + \frac{\hbar}{2m} \sum_{\lambda} \Psi^{r\lambda}_{q^{r\lambda}} - v(r)\Psi^0 = 0,$$

with the contact conditions

$$\Delta^{c\alpha} \equiv \Psi^0_{q^{c\alpha}} - \Psi^{c\alpha} = 0,$$

$$\Delta^{r\lambda} \equiv \Psi^0_{q^{r\lambda}} - \Psi^{r\lambda} = 0.$$

We have written the physicist’s version of the equation, keeping the Planck’s constant, the relevant masses and the imaginary number $i$. We use a compact notation $q^a$, $a = 0,$
contact symmetry of time-dependent Schrödinger equation 53

cα, rλ, where q^0 = t, q^{cα} = R_α, q^{rλ} = r_λ. Here and later on α, λ etc. will mean the
cartesian components, subscripted variables (other than the cartesian components) will
mean derivatives with respect to those subscripts, the letters c and r will mean center-of-
mass and relative coordinates, and t will mean time.

Equations (2), (3) are actually the definitions of the gradient variables. The inter-
particle potential v(r) has been taken to be of central nature. In terms of the gradient
variables the Schrödinger equation is now of the first or

der.

The generators of the Lie group transformations in the space of q^a, Ψ^a are of the form

X = \sum_a \left[ \xi^a(q, Ψ) \frac{∂}{∂q^a} + \chi^a(q, Ψ) \frac{∂}{∂Ψ^a} \right],

(4)

with a = 0, cα, rλ. The arguments of ξ^a and χ^a contain the collection of all q^a and Ψ^a. In
the Racah nomenclature the ξs and χs are called the velocity vectors of the generator X. If
χ^0 explicitly contains the gradients Ψ^{cα}, Ψ^{rλ}, then the contact transformation is essentially
different from a point transformation [2].

As in the case of point transformations, the first extention of X is written as

X^{(1)} = X + \sum_{a,b} \chi^{a;b} \frac{∂}{∂Ψ^a}.

(5)

Here,

\chi^{a;b} = \chi^b_{q^a} - \sum_{b'} Ψ^a_{q^{b'}} ξ^{b'}_{q^{b'}} - \sum_{a',b'} Ψ^{a'}_{q^{a'}} Ψ^a_{q^{b}} ξ^{b'}_{q^{b'}} + \sum_{a'} Ψ^{a'}_{q^{a'}} χ^a_{q^{a'}}.

(6)

The effect of X^{(1)} on the different ∆s of equations (1), (2), (3) are

X^{(1)} ∆^0 ≡ iχ^{0,t} + \hbar \sum_α \chi^{cα,cα} + \hbar \sum_λ \chi^{rλ,rλ} - v(r)χ^0 - \frac{v(r)'}{r} \sum_λ ξ^{rλ,rλ} Ψ = 0, \quad (7)

X^{(1)} ∆^{cα} ≡ ξ^{0;cα} - χ^{cα} = 0, \quad (8)

X^{(1)} ∆^{rλ} ≡ ξ^{0;rλ} - χ^{rλ} = 0.

3  Defining equations of group generators

The group of contact transformations for the equation (1) will be uniquely known when the
velocity vectors ξ^a and χ^a will be obtained. These velocity vectors satisfy an overcomplete
set of differential equations known as the defining equations. These defining equations
are obtained by separately equating to zero the coefficients of the different monomials in
Ψ^a, appearing in equations (1), (3), (4).

In our case we get the defining relations:

ξ^{0}_{ψ^{cα}} ≡ ξ^{0}_{ψ^{rλ}} = 0, \quad (10)

ξ^{0}_{ψ^{cα}} + Ψ^{cα} ξ^{0}_{ψ} ≡ ξ^{0}_{ψ^{rλ}} + Ψ^{rλ} ξ^{0}_{ψ} = 0, \quad (11)

ξ^{cα}_{ψ^{rλ}} ≡ ξ^{rλ}_{ψ^{cα}} = 0, \quad (12)
\[
\frac{1}{M} \delta_{\alpha\beta} \varepsilon_{r\mu} + \frac{1}{m} \delta_{\lambda\mu} \varepsilon_{\psi,0} = 0, \\
\delta_{\nu\lambda} \xi_{q,\psi} + \delta_{\sigma\mu} \xi_{r\nu\lambda} = 0, \\
\delta_{\gamma\alpha} \xi_{q,\psi} + \delta_{\sigma\beta} \xi_{r\gamma\psi} = 0, \\
\chi_{\psi,0}^0 - \sum_{\beta} \Psi_{\beta,\psi} \chi_{q,\psi}^0 - \sum_{\mu} \Psi_{r\mu,\psi} \xi_{\psi,0}^0 = 0, \\
\chi_{\psi,\psi}^0 - \sum_{\beta} \Psi_{\beta,\psi} \chi_{q,\psi}^0 - \sum_{\mu} \Psi_{r\mu,\psi} \xi_{\psi,\psi}^0 = 0, \\
\left[ \chi_{\psi,\psi}^0 - \sum_{\beta} \Psi_{\beta,\psi} \chi_{q,\psi}^0 - \sum_{\mu} \Psi_{r\mu,\psi} \xi_{\psi,\psi}^0 \right] + \Psi_{r,\psi}^0 - \chi_{\psi,\psi}^0 = 0, \\
\left[ \chi_{\psi,\psi}^0 - \sum_{\beta} \Psi_{\beta,\psi} \chi_{q,\psi}^0 - \sum_{\mu} \Psi_{r\mu,\psi} \xi_{\psi,\psi}^0 \right] + \Psi_{r,\psi}^0 = 0, \\
\frac{\hbar}{2M} \chi_{\psi,\psi}^0 + \frac{\hbar}{2m} \left[ \chi_{\psi,\psi}^0 + \Psi_{r,\psi} \chi_{\psi,\psi}^0 \right] = 0, \\
\frac{\hbar}{2m} \chi_{\psi,\psi}^0 + \frac{\hbar}{2M} \left[ \chi_{\psi,\psi}^0 + \Psi_{r,\psi} \chi_{\psi,\psi}^0 \right] = 0, \\
i \left[ \chi_{\psi,\psi}^0 - \sum_{\beta} \Psi_{\beta,\psi} \chi_{q,\psi}^0 - \sum_{\mu} \Psi_{r\mu,\psi} \xi_{\psi,\psi}^0 \right] + v(r) \Psi^0 \left[ \chi_{\psi,\psi}^0 - \sum_{\beta} \Psi_{\beta,\psi} \chi_{q,\psi}^0 - \sum_{\mu} \Psi_{r\mu,\psi} \xi_{\psi,\psi}^0 \right] \\
+ \frac{\hbar}{2M} \sum_{\alpha} \left[ \chi_{\psi,\psi}^0 + \Psi_{r,\psi} \chi_{\psi,\psi}^0 \right] + \frac{\hbar}{2M} \sum_{\lambda} \left[ \chi_{\psi,\psi}^0 + \Psi_{r,\psi} \chi_{\psi,\psi}^0 \right] \\
- v(r) \left[ \chi_{\psi,\psi}^0 + \Psi_{r,\psi} \chi_{\psi,\psi}^0 \right] + \frac{v(r)}{r \Psi^0} \Psi^0 \sum_{\lambda} r_{\lambda} \xi_{r\lambda}^0 \right] = 0.
\]
We have obtained the general solution of these defining equations and have indicated the method in the Appendix 1. The velocity vectors are expressed in terms of the auxiliary functions

$$F_0(t, \vec{R}, \vec{r}) = A_0(t) - \frac{iM}{\hbar} \sum_{\alpha} f_0^{\alpha}(t) R_\alpha - \frac{im}{\hbar} \sum_{\lambda} f_0^{\lambda}(t) r_\lambda$$

$$+ \frac{iM}{4\hbar} b(t)^{''} \sum_{\alpha} R_\alpha^2 + \frac{im}{\hbar} b(t)^{''} \sum_{\lambda} r_\lambda^2,$$

$$F^{\alpha}(t, \vec{R}, \vec{r}) = f_0^{\alpha}(t) - \frac{1}{2} b(t)^{'} R_\alpha + \sum_{\beta\gamma} e_{\alpha\beta\gamma} f^{\gamma}_{1} R_\beta + m \sum_{\lambda} f_0^{\alpha\gamma\lambda} r_\lambda,$$

$$F^{\lambda}(t, \vec{R}, \vec{r}) = f_0^{\lambda}(t) - \frac{1}{2} b(t)^{'} r_\lambda + \sum_{\mu\nu} e_{\lambda\mu\nu} f^{\nu}_{1} r_\mu - M \sum_{\alpha} f_0^{\alpha\nu\nu} R_\alpha,$$

and are of the form

$$\xi_0(t) = b(t),$$

$$\xi^{\alpha}(t, \vec{R}, \vec{r}) = -F^{\alpha}(t, \vec{R}, \vec{r}),$$

$$\xi^{\lambda}(t, \vec{R}, \vec{r}) = -F^{\nu}(t, \vec{R}, \vec{r}),$$

$$\chi_0(t, \vec{R}, \vec{r}, \Psi^0) = f_0^0(t, \vec{R}, \vec{r}) + \Psi^0,$$

$$\chi^{\alpha}(t, \vec{R}, \vec{r}, \Psi^0) = \frac{\partial \chi_0(t, \vec{R}, \vec{r}, \Psi^0)}{\partial R_\alpha} - M \sum_{\lambda} \Psi^{\nu\lambda} f_0^{\alpha\nu\nu},$$

$$\chi^{\lambda}(t, \vec{R}, \vec{r}, \Psi^0) = \frac{\partial \chi_0(t, \vec{R}, \vec{r}, \Psi^0)}{\partial r_\lambda} + m \sum_{\alpha} \Psi^{\alpha\lambda} f_0^{\alpha\lambda},$$

where $F^0(t, \vec{R}, \vec{r})$ and $f^0(t, \vec{R}, \vec{r})$ satisfy

$$i \frac{\partial F^0(t, \vec{R}, \vec{r})}{\partial t} + \frac{\hbar}{2M} \sum_\alpha \frac{\partial^2 F^0(t, \vec{R}, \vec{r})}{(\partial R_\alpha)^2} + \frac{\hbar}{2m} \sum_\lambda \frac{\partial^2 F^0(t, \vec{R}, \vec{r})}{(\partial r_\lambda)^2}$$

$$- v(r) b(t)^{'} + \frac{v(r)^{'} r_\lambda}{r} F^{\nu\lambda}(t, \vec{R}, \vec{r}) = 0,$$

$$i \frac{\partial f^0(t, \vec{R}, \vec{r})}{\partial t} + \frac{\hbar}{2M} \sum_\alpha \frac{\partial^2 f^0(t, \vec{R}, \vec{r})}{(\partial R_\alpha)^2} + \frac{\hbar}{2m} \sum_\lambda \frac{\partial^2 f^0(t, \vec{R}, \vec{r})}{(\partial r_\lambda)^2}$$

$$- v(r) f^0(t, \vec{R}, \vec{r}) = 0.$$
| Name/ Symbol of the generator | Form of the generator |
|------------------------------|-----------------------|
| **Scaling**: $X_S$ | $\Psi^0 \frac{\partial}{\partial \Psi^0} + \sum_\alpha \Psi^{\alpha} \frac{\partial}{\partial \Psi^{\alpha}} + \sum_\lambda \Psi^{\lambda} \frac{\partial}{\partial \Psi^{\lambda}}$ |
| **time translation**: $X^t$ | $i \frac{\partial}{\partial t}$ |
| **centre of mass coordinate**
| **space translations**: $X_T^{\alpha}$ | $-i \frac{\partial}{\partial R_\alpha}$ |
| **relative coordinate**
| **space translations**: $X_T^{\lambda}$ | $-i \frac{\partial}{\partial r_\lambda}$ |
| **centre of mass coordinate**
| **Galilean transformations**: $X_G^{\alpha}$ | $tX_T^{\alpha} + \frac{M}{\hbar} \left( R_\alpha X_S + \Psi^0 \frac{\partial}{\partial \Psi^{\alpha}} \right)$ |
| **relative coordinate**
| **Galilean transformations**: $X_G^{\lambda}$ | $tX_T^{\lambda} + \frac{m}{\hbar} \left( r_\lambda X_S + \Psi^0 \frac{\partial}{\partial \Psi^{r\lambda}} \right)$ |
| **centre of mass coordinate**
| **space rotations**: $X_R^{\alpha}$ | $-i \sum_\beta e_{\alpha \beta \gamma} \left( R_\beta \frac{\partial}{\partial R_\gamma} + \Psi^{\beta} \frac{\partial}{\partial \Psi^{\gamma}} \right)$ |
| **relative coordinate**
| **space rotations**: $X_R^{\lambda}$ | $-i \sum_\mu e_{\lambda \mu \nu} \left( R_\mu \frac{\partial}{\partial r_\nu} + \Psi^{r\mu} \frac{\partial}{\partial \Psi^{r\nu}} \right)$ |
| **cross-rotations**: $X_R^{\alpha \lambda}$ | $-i \sqrt{\frac{m}{M}} \left( \rho_\lambda \frac{\partial}{\partial R_\alpha} - \Psi^{\alpha} \frac{\partial}{\partial \Psi^{r\lambda}} \right) + i \sqrt{\frac{M}{m}} \left( \rho_\alpha \frac{\partial}{\partial r_\lambda} - \Psi^{r\alpha} \frac{\partial}{\partial \Psi^{r\lambda}} \right)$ |
| | $X_1$ | $2tX^t - \sum_\alpha R_\alpha X_T^{\alpha} - \sum_\lambda r_\lambda X_T^{\lambda} + 2v_0 tX_S + i\Psi^0 \frac{\partial}{\partial \Psi^0}$ |
| | $X_2$ | $i^2 X^t + \sum_\alpha R_\alpha X_T^{\alpha} - i \sum_\lambda r_\lambda X_T^{\lambda}$ |
| | | $- \left[ \frac{M}{2\hbar} \sum_\alpha R_\alpha^2 + \frac{m}{2\hbar} \sum_\lambda r_\lambda^2 + 4it - v_0 t \right] X_S$ |
| | | $- \Psi^0 \left[ -i \frac{\partial}{\partial \Psi^0} + \frac{M}{\hbar} \sum_\alpha R_\alpha \frac{\partial}{\partial \Psi^{\alpha}} + \frac{m}{\hbar} \sum_\lambda r_\lambda \frac{\partial}{\partial \Psi^{r\lambda}} \right]$ |
| **relative vibrations**: $X_{\chi(\pm)}^{\lambda}$ | $e^{\pm i\omega t} \left[ -i \frac{\partial}{\partial r_\lambda} \pm \frac{im \omega}{\hbar} r_\lambda X_S \pm \frac{im \omega}{\hbar} \Psi^0 \frac{\partial}{\partial \Psi^{r\lambda}} \right]$ |

Table 1. Generators that describe the different Lie Algebras of the four classes of inter-particle potential.

Here, a prime on the function of a single variable denotes derivative with respect to that variable, $e_{\alpha \beta \gamma}$ and $e_{\lambda \mu \nu}$ are the permutation symbols and $f_1^{\alpha}$, $f_1^{\lambda}$, $f_0^{\alpha \lambda}$ are constants. Since $\chi^0(t, \vec{R}, \vec{r}; \Psi^0)$ does not contain $\Psi^{\alpha}$ and $\Psi^{\lambda}$, the group of contact transformations for this system is not essentially different from that of point transformations. However, the generators now contain derivatives with respect to the gradient variables, because the
group of contact transformations is the first extension of the group of point transformations.

Equation (35) is nothing but the original Schrödinger equation and \( f^0(t, \vec{R}, \vec{r}) \) is a solution of equation (1). This is the symmetry corresponding to linear superposition principle of the Schrödinger equation and forms an infinite dimensional invariant subgroup of the total group. The factor group modulo this subgroup is the physical group of interest and will be referred to as the group of contact transformations.

Substituting \( F^0(t, \vec{R}, \vec{r}) \) from equation (25) in equation (34) and equating coefficients of different monomials in the space coordinates to zero, we get

\[
b(t)^n = 0, \tag{36}
\]
\[
f^{c\alpha}_0(t)^n = 0, \tag{37}
\]
\[
\frac{m}{\hbar} f^{r\lambda}_0(t)^n + \frac{v(r)'}{r} f^{r\lambda}_0(t) = 0, \tag{38}
\]
\[
iA_0(t)' + \frac{3i}{2} b(t)^n - \left[ v(r) + \frac{1}{2} rv(r)' \right] b(t)' = 0, \tag{39}
\]
and either
\[
v(r)' = 0 \tag{40}
\]
or
\[
f^{c\alpha;r\lambda}_0 = 0. \tag{41}
\]

4 Symmetry classification of interparticle potentials

From the solution of equations (36)–(41) we get four different classes of interparticle potentials. This complete symmetry analysis of the 2-particle Schrödinger equation as far as the dynamics of the system is concerned shows that contact transformations do not enforce any more restriction than that already required on the basis of point transformation symmetry of the system. Their group algebras are the first extensions of the algebras of point transformation symmetries of the corresponding potentials [6].

These group algebras are described in terms of the generators given in Table 1.

The letters \( T, G, R \) and \( V \) in the symbols of the generators denote space translational, galilean, space rotational and vibrational modes described by these generators. We have kept the imaginary number \( i \) in the forms of the generators so that these can be identified with the usual quantum mechanical operators for energy, linear and angular momenta.

In actual calculations with the group algebras, the structure constants (commutation relations in physicists’ parlance) are of the greatest help. They are given in Appendix 2.

Any Lie Algebra \( L \) is a semi-direct product of its Radical \( R \) and a semisimple part \( L/R \). The semisimple part \( L/R \) is again a direct sum of ideals which, as subalgebras, are simple [6, 8]. These characteristics of the Lie Algebras for the different classes of inter-particle potentials are given in Table 2.

It is to be noted that the generators for the space translational and Galilean as well as vibrational transformations always belong to the Radical of the Lie Algebra.
Table 2. Characteristics of the Lie Algebras of the Symmetry groups of the different classes of inter-particle potential.

| Inter-particle potential: $v(r)$ | Constant | Harmonic oscillator | Inverse square | Arbitrary |
|----------------------------------|----------|---------------------|---------------|----------|
| $v(r)$                           | $v_0$    | $v_0 + \frac{m\omega^2 r^2}{2\hbar}$ | $v_0 - \frac{v_1}{r^2}$ | $\neq v_0$, $v_0 + \frac{m\omega^2 r^2}{2\hbar}$, $v_0 - \frac{v_1}{r^2}$ |

| Generators of Lie Algebra, $L$ | $\{X_S, X^c, X^{\alpha}_{G,T,R} \}$ | $\{X_S, X^c, X^{\alpha}_{G,T,R} \}$ | $\{X_S, X^c, X^{\alpha}_{G,T,R} \}$ | $\{X_S, X^c, X^{\alpha}_{G,T,R} \}$ |

| Dimension | 31 | 20 | 16 | 14 |

| Solvability, Nilpotency, Simplicity, Semisimplicity | None | None | None | None |

| Centre, $Z(L)$ | $\{X_S \}$ | $\{X_S \}$ | $\{X_S \}$ | $\{X_S \}$ |

| Radical, $R$ | $\{X_S, X^{c,\alpha}_{G,T}, X^{\alpha}_{G,T} \}$ | $\{X_S, X^{c,\alpha}_{G,T}, X^{\alpha}_{G,T} \}$ | $\{X_S, X^{c,\alpha}_{G,T} \}$ | $\{X_S, X^{c,\alpha}_{G,T} \}$ |

| Semisimple part as direct sum $L/R = \sum_i \circlearrowleft I_i$ of simple ideals | $I_1 = \{X^c, X_1, X_2 \}$, $I_2 = \{X^c, X_R, X^{\alpha}_{G,T} \}$, $I_3 = \{X_R \}$ | $I_1 = \{X^c, X_1, X_2 \}$, $I_2 = \{X^c, X_R, X^{\alpha}_{G,T} \}$, $I_3 = \{X_R \}$ | $I_1 = \{X^c, X_1, X_2 \}$, $I_2 = \{X^c, X_R, X^{\alpha}_{G,T} \}$, $I_3 = \{X_R \}$ | $I_1 = \{X^c, X_1, X_2 \}$, $I_2 = \{X^c, X_R, X^{\alpha}_{G,T} \}$, $I_3 = \{X_R \}$ |

| Cartan subalgebra $H$ | $\{X_S, X^c, X^{c,\alpha}_{R}, X^{\alpha}_{G,T,R} \}$ | $\{X_S, X^c, X^{c,\alpha}_{R}, X^{\alpha}_{G,T,R} \}$ | $\{X_S, X^c, X^{c,\alpha}_{R}, X^{\alpha}_{G,T,R} \}$ | $\{X_S, X^c, X^{c,\alpha}_{R}, X^{\alpha}_{G,T,R} \}$ |

We note that the Radical, being solvable, has only 1-dimensional irreducible representations (irreps). Thus the irreps of $L$ are obtained if the irreps of $L/R$ are known. To this end we give in Table 3 the algebraic characteristics of the simple subalgebras appearing in the direct sum of $L/R$ for the different classes of inter-particle potential.

## 5 Functional bases of invariants

In order to investigate integrability of a dynamical system we require the functional bases of invariants in terms of which all invariants of the dynamical system can be expressed functionally. These base invariants of a Lie algebra $L$ generate the Centre of the Universal Enveloping algebra of $L$. Since they commute with all the generators of $L$, they appear as conserved quantities of the system. Lie’s method has been utilized to obtain the base invariants for the four symmetry groups of Section 4. If the functional base has $s$ invariants $I_1, I_2, \ldots, I_s$, each a function of the $r$ generators $X_a$ of the symmetry group, then

$$[X_a, I_b] = 0, \quad a = 1, \ldots, r, \quad b = 1, \ldots, s.$$
Contact Symmetry of Time-Dependent Schrödinger Equation

| Algebra: \( L \) | \( L_1 \) | \( L_2 \) | \( L_3 \) | \( L_4 \) |
|-----------------|----------|----------|----------|----------|
| Generators: \( \{X_i\} \) | \( \{X^t, X_1, X_2\} \) | \( \{X^c_{\alpha}, X^r_{\lambda}, X^{c;\alpha;r;\lambda}\} \) | \( \{X_R^3\} \) | \( \{X^t\} \) |
| Dimension | 3 | 15 | 3 | 1 |
| Cartan subalgebra: \( H \) | \( \{-\frac{i}{2}X_1\} \) | \( \{X^c_3, X^r_3, X^{c;3;r;3}\} \) | \( \{X^3_R\} \) | \( \{X^t\} \) |
| Rank | 1 | 3 | 1 | 1 |
| Base of simple roots: \( \Delta \) | \( \alpha = 1 \) | \( \alpha_1 = \begin{pmatrix} -1 \\ 0 \\ -1 \end{pmatrix} \), \( \alpha_2 = \begin{pmatrix} -1 \\ 0 \\ 1 \end{pmatrix} \), \( \alpha_3 = \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix} \) | \( \alpha = 1 \) | void |
| Root system | \( \pm \alpha \) | \( \pm \alpha_1, \pm \alpha_2, \pm \alpha_3, \) | \( \pm (\alpha_1 + \alpha_3), \pm (\alpha_2 + \alpha_3), \) | \( \pm \alpha \) | void |
| Isomorphy to | \( O(3) \) | \( O(6) \) | \( O(3) \) | \( U(1) \) |

Table 3. Characteristics of the simple subalgebras forming the semisimple parts in Table 2.

If \( I \) is any other invariant so that
\[
[X_a, I] = 0, \quad a = 1, \ldots, r,
\]
then \( I \) can be functionally expressed as
\[
I \equiv I(I_1, \ldots, I_s).
\]

If the base has the constant as its only member, then the system is completely chaotic. If on the other hand \( s = r \) and all the generators give mutually commuting invariants, then the system is fully integrable. Actual dynamical systems are almost always in between...
these two extreme cases. In the four symmetry classes obtained in Section 4, the same thing happens.

In Table 4 we define auxiliary operators in terms of which the functional bases of invariants for the four classes of distinct inter-particle potentials are given in Table 5.

| Inter-particle potential | Auxiliary operators |
|--------------------------|---------------------|
| Constant potential       | $Y^c_R = X_S X^c_R + \frac{\hbar}{M} \sum_{\beta\gamma} e_{\alpha\beta\gamma} X^c_T X^c_G$, $Y^r_R = X_S X^r_R + \frac{\hbar}{m} \sum_{\mu\nu} e_{\lambda\mu\nu} X^r_T X^r_G$, $Y^{c\alpha\gamma} = X_S X^{c\alpha\gamma} + \frac{\hbar}{\sqrt{mM}} \left[ X^c_G X^r_T - X^r_G X^c_T \right]$, $Y^t = X_S X^t + v_0 (X_S)^2 + \frac{\hbar}{2M} \sum_{\alpha} (X^c_T)^2 + \frac{\hbar}{2m} \sum_{\lambda} (X^r_T)^2$, $Y_1 = X_S X_1 - 4i (X_S)^2 + \frac{\hbar}{M} \sum_{\alpha} X^c_T X^c_G + \frac{\hbar}{m} \sum_{\lambda} X^r_T X^r_G$, $Y_2 = X_S X_2 + \frac{\hbar}{2M} \sum_{\alpha} (X^c_G)^2 + \frac{\hbar}{2m} \sum_{\lambda} (X^r_G)^2$ |
| Harmonic oscillator potential | $Y^c_R = X_S X^c_R + \frac{\hbar}{M} \sum_{\beta\gamma} e_{\alpha\beta\gamma} X^c_T X^c_G$, $Y^r_R = X_S X^r_R + \frac{ih}{2m\omega} \sum_{\mu\nu} e_{\lambda\mu\nu} X^r_T X^r_G$, $Y^t = X_S X^t + \frac{\hbar}{2M} \sum_{\alpha} (X^c_T)^2 + \frac{\hbar}{2m} \sum_{\lambda} X^r_T X^r_G$, $Y_1 = X_S X_1 - 4i (X_S)^2 + \frac{\hbar}{M} \sum_{\alpha} X^c_T X^c_G$, $Y_2 = X_S X_2 + \frac{\hbar}{2M} \sum_{\alpha} (X^c_G)^2$ |
| Inverse square potential | $Y^c_R = X_S X^c_R + \frac{\hbar}{M} \sum_{\beta\gamma} e_{\alpha\beta\gamma} X^c_T X^c_G$, $Y^t = X_S X^t + v_0 (X_S)^2 + \frac{\hbar}{2M} \sum_{\alpha} (X^c_T)^2$, $Y_1 = X_S X_1 - 4i (X_S)^2 + \frac{\hbar}{M} \sum_{\alpha} X^c_T X^c_G$, $Y_2 = X_S X_2 + \frac{\hbar}{2M} \sum_{\alpha} (X^c_G)^2$ |
| Arbitrary potential | $Y^c_R = X_S X^c_R + \frac{\hbar}{M} \sum_{\beta\gamma} e_{\alpha\beta\gamma} X^c_T X^c_G$, $Y^t = X_S X^t + \frac{\hbar}{2M} \sum_{\alpha} (X^c_T)^2$ |

Table 4. Auxiliary operators for the four distinct classes of inter-particle potentials.

In all these cases $I_S$ is the scaling operator and $I^t$ is essentially the energy operator, $I^c_R$ and $I^r_R$ are the c.m.coordinate and the relative coordinate angular momentum operators. Except for the case of constant potential, these are the only invariants. The only potential that has more invariants is the constant potential and the two extra invariants $I^c_3$ and $I^c_4$ of degrees 3 and 4 in the generators make this apparently simple system actually more complicated yet more systematic.
| Inter – particle potential | Base Invariants |
|---------------------------|----------------|
| **Constant potential**    | $I_S = X_S$,   |
|                           | $I^t = Y^t$,   |
|                           | $I^0_R = \sum_\alpha (Y^{ca\alpha})^2 + \sum_\lambda (Y^{t\lambda})^2 + \sum_{\alpha\lambda} (Y^{ca\alpha;\lambda})^2$, |
|                           | $I_{3R}^c = \sum_{\alpha\lambda} Y^{ca\alpha} Y^{ca\alpha;\lambda} Y^{t\lambda}$ |
|                           | $-\frac{1}{6} \sum_{\alpha\beta\gamma\lambda\mu\nu} e_{\alpha\beta\gamma} e_{\lambda\mu\nu} Y^{ca\alpha;\lambda} Y^{ca\beta;\mu} Y^{ca\gamma;\nu}$ |
|                           | $I_{4R}^c = \left[ \sum_\alpha (Y^{ca\alpha})^2 \right] \left[ \sum_\lambda (Y^{t\lambda})^2 \right]$ |
|                           | $+ \sum_\alpha \left[ \sum_\lambda Y^{ca\alpha;\lambda} Y^{t\lambda} \right]^2 + \sum_\lambda \left[ \sum_\alpha Y^{ca\alpha} Y^{ca;\lambda} \right]^2$ |
|                           | $+ \frac{1}{2} \sum_\alpha \left[ \sum_{\beta\gamma} \sum_{\mu\nu} e_{\alpha\beta\gamma} e_{\lambda\mu\nu} Y^{ca\beta;\mu} Y^{ca\gamma;\nu} \right]^2$ |
|                           | $- \sum_\alpha Y^{c\alpha} \left[ \sum_{\beta\gamma} \sum_{\mu\nu} e_{\alpha\beta\gamma} e_{\lambda\mu\nu} Y^{ca\beta;\mu} Y^{ca\gamma;\nu} \right] Y^{t\lambda}$ |
| **Harmonic oscillator**   | $I_S = X_S$,   |
|                           | $I^t = Y^t$,   |
|                           | $I^0_R = \sum_\alpha (Y^{ca\alpha})^2$, |
|                           | $I_{3R}^c = \sum_\alpha (Y^{ca\alpha})^2$, |
|                           | $I_{4R}^c = \sum_\alpha (Y^{ca\alpha})^2$, |
| **Inverse square potential** | $I_S = X_S$,   |
|                           | $I^t = Y^t$,   |
|                           | $I^0_R = \sum_\alpha (Y^{ca\alpha})^2$, |
|                           | $I_{3R}^c = \sum_\alpha (Y^{ca\alpha})^2$, |
|                           | $I_{4R}^c = \sum_\alpha (X^{t\lambda})^2$, |
| **Arbitrary potential**   | $I_S = X_S$,   |
|                           | $I^t = Y^t$,   |
|                           | $I^0_R = \sum_\alpha (Y^{ca\alpha})^2$, |
|                           | $I_{3R}^c = \sum_\alpha (Y^{ca\alpha})^2$, |
|                           | $I_{4R}^c = \sum_\alpha (X^{t\lambda})^2$, |

Table 5. Functional base of invariants for the different classes of inter-particle potentials.

It is to be noted that in all the expressions in this section involving products of operators symmetrized forms have to be taken.

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In this Appendix we indicate how the defining equations (10)–(24) are solved to obtain
the group generators.

Equations (10), (11) give
\[ \xi^0 \equiv \xi^0(t). \]
From equations (12)–(15) it follows that
\[ \xi^{c\alpha} \equiv \xi^{c\alpha}(t, \vec{R}, \vec{r}, \Psi^0), \quad \xi^{r\lambda} \equiv \xi^{r\lambda}(t, \vec{R}, \vec{r}, \Psi^0). \] (42)

Equations (16), (17) thus give
\[ \chi^0 \equiv \chi^0(t, \vec{R}, \vec{r}, \Psi^0). \] (43)

Using the auxiliary function
\[ F(q^a, \Psi^a) = \chi^0 - \sum_\alpha \Psi^{c\alpha} \xi^{c\alpha} - \sum_\lambda \Psi^{r\lambda} \xi^{r\lambda}, \] (44)
equations (18) and (19) now become
\[ \xi^{c\alpha} = -\frac{\partial F}{\partial \Psi^{c\alpha}}, \] (45)
\[ \xi^{r\lambda} = -\frac{\partial F}{\partial \Psi^{r\lambda}}, \] (46)
\[ \chi^{c\alpha} = \frac{\partial F}{\partial q^{c\alpha}} + \Psi^{c\alpha} \frac{\partial F}{\partial \Psi^0}, \] (47)
\[ \chi^{r\lambda} = \frac{\partial F}{\partial q^{r\lambda}} + \Psi^{r\lambda} \frac{\partial F}{\partial \Psi^0}, \] (48)
\[ \chi^0 = F - \sum_\alpha \Psi^{c\alpha} \frac{\partial F}{\partial \Psi^{c\alpha}} - \sum_\lambda \Psi^{r\lambda} \frac{\partial F}{\partial \Psi^{r\lambda}}. \] (49)

Here \( F \) is linear in \( \Psi^{c\alpha} \) and \( \Psi^{r\lambda} \). Because of this linearity, equations (18)–(21) give
\[ \xi^{c\alpha} \equiv \xi^{c\alpha}(t, \vec{R}, \vec{r}), \quad \xi^{r\lambda} \equiv \xi^{r\lambda}(t, \vec{R}, \vec{r}), \] (50)
and equations (14), (17), (18) and (50) imply linearity of \( \chi^{c\alpha} \) and \( \chi^{r\lambda} \) with respect to \( \Psi^{c\alpha} \) and \( \Psi^{r\lambda} \). Equations (20), (21) together with equations (14)–(18) now give
\[ \xi^{c\alpha} + \xi^{\beta c\alpha} = \delta_{\alpha\beta} \xi^{0c\alpha}, \]
\[ \xi^{r\lambda} + \xi^{r\lambda} = \delta_{\lambda\mu} \xi^{0r\lambda}, \] (51)
and equations (22), (23) become
\[ m \xi^{r\lambda} + M \xi^{c\alpha} = 0. \] (52)

From equation (24) equating separately to zero terms quadratic in, linear in and independent of \( \Psi^{c\alpha} \) and \( \Psi^{r\lambda} \), we get
\[ \chi_{\Psi^0, \Phi^0}^0 = 0, \] (53)
Equations (63) and (64) are obtained from the terms that are linear in and independent of $\Psi^0$ in equation (60). Equation (63) gives us the result that $F^\alpha\lambda$ is linear in $\vec{R}$; and equation (64) shows that $F^\nu\lambda$ is linear in $\vec{r}$. Equation (61) will now give $F^0$, $F^\alpha\lambda$ and $F^\nu\lambda$ as in equations (51)–(57) and (62)–(68) and the difference is that $f^\gamma_0$, $f^\nu_0$ and $f^\alpha\lambda_0$ are yet functions of time $t$. Equations (61), (62) now ensure that these are indeed independent of $t$.

From equation (63) we also obtain equations (66)–(71).
In this Appendix we give the structure constants of the generators given in Table 1.

\[
[X^t, X_G^\alpha] = iX_T^\alpha, \quad [X^t, X_G^{r\lambda}] = iX_T^{r\lambda}, \quad [X^t, X_1] = 2i(X^t + v_0X_S),
\]

\[
[X^t, X_2] = iX_1 + 4X_S, \quad [X_G^{c\alpha}, X_G^{c\beta}] = -\frac{iM}{\hbar}\delta_{\alpha\beta}X_S,
\]

\[
[X_T^{c\alpha}, X_R^{c\beta}] = i\sum_\gamma e_{\alpha\beta\gamma}X_T^{c\gamma}, \quad [X_T^{c\alpha}, X_1] = iX_T^{c\alpha}, \quad [X_T^{c\alpha}, X_2] = iX_G^{c\alpha},
\]

\[
[X_T^{c\alpha}, X_G^{c\beta;r\lambda}] = i\sqrt{\frac{M}{m}}\delta_{\alpha\beta}X_T^{r\lambda}, \quad [X_T^{c\alpha}, X_R^{c\beta}] = i\sum_\gamma e_{\alpha\beta\gamma}X_G^{c\gamma},
\]

\[
[X_G^{c\alpha}, X_1] = -iX_G^{c\alpha}, \quad [X_G^{c\alpha}, X_G^{c\beta;r\lambda}] = i\sqrt{\frac{M}{m}}\delta_{\alpha\beta}X_G^{r\lambda},
\]

\[
[X_R^{c\alpha}, X_R^{c\beta}] = i\sum_\gamma e_{\alpha\beta\gamma}X_R^{c\gamma}, \quad [X_R^{c\alpha}, X_R^{c\beta;r\lambda}] = i\sum_\gamma e_{\alpha\beta\gamma}X_R^{c\gamma;r\lambda},
\]

\[
[X_T^{r\lambda}, X_T^{r\mu}] = -\frac{im}{\hbar}\delta_{\lambda\mu}X_S, \quad [X_T^{r\lambda}, X_R^{r\mu}] = i\sum_\nu e_{\lambda\mu\nu}X_T^{r\nu},
\]

\[
[X_T^{r\lambda}, X_1] = iX_T^{r\lambda}, \quad [X_T^{r\lambda}, X_2] = iX_G^{r\lambda}, \quad [X_T^{r\lambda}, X_G^{c\alpha;r\mu}] = -\sqrt{\frac{m}{M}}\delta_{\lambda\mu}X_T^{c\alpha},
\]

\[
[X_G^{r\lambda}, X_G^{r\mu}] = i\sum_\nu e_{\lambda\mu\nu}X_G^{r\nu}, \quad [X_G^{r\lambda}, X_1] = -iX_G^{r\lambda},
\]

\[
[X_G^{r\lambda}, X_G^{c\alpha;r\mu}] = -\sqrt{\frac{m}{M}}\delta_{\lambda\mu}X_G^{c\alpha},
\]

\[
[X_R^{r\lambda}, X_R^{r\mu}] = i\sum_\nu e_{\lambda\mu\nu}X_R^{r\nu}, \quad [X_R^{r\lambda}, X_G^{c\alpha;r\mu}] = i\sum_\nu e_{\lambda\mu\nu}X_G^{c\alpha;r\nu},
\]

\[
[X_G^{c\alpha;r\lambda}, X_G^{c\beta;r\mu}] = i\left(\delta_{\alpha\beta}\sum_\nu e_{\lambda\mu\nu}X_R^{r\nu} + \delta_{\lambda\mu}\sum_\gamma e_{\alpha\beta\gamma}X_R^{c\gamma}\right),
\]

\[
[X_1, X_2] = 2iX_2, \quad [X^t, X_{V(\pm)}^{r\lambda}] = \mp\omega X_{V(\pm)}^{r\lambda},
\]

\[
[X_R^{r\lambda}, X_{V(\pm)}^{r\mu}] = i\sum_\nu e_{\lambda\mu\nu}X_{V(\pm)}^{r\nu}, \quad [X_{V(\pm)}^{r\lambda}, X_{V(\pm)}^{r\mu}] = -\frac{2m\omega}{\hbar}\delta_{\lambda\mu}X_S.
\]
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