DISTANCE-DEPENDENT INTERACTIONS AND SYMMETRY CONSERVATION IN MULTI-PARTICLE SYSTEM

[1]Ashuthosh,[2]Sudharshan
[1234]Students
Department of H&S

ABSTRACT:

In many-body physics, understanding how symmetry principles govern system dynamics is fundamental to both classical and quantum mechanical formulations. This study focuses on multi-particle systems with pairwise distance-dependent interaction potentials, exploring the emergence and conservation of spatial and dynamical symmetries. Using analytical techniques and group-theoretical methods, we examine how the form of the potential—dependent solely on inter-particle distances—affects invariants such as momentum, angular momentum, and total energy. The work highlights the connection between spherically symmetric potentials and global symmetry groups, including translational and rotational invariance. Applications range from gravitational and Coulombic systems to molecular and condensed matter models. The study underscores the critical role of potential symmetry in defining conserved quantities, integrability, and system behavior under perturbation.

INTRODUCTION

The dynamics of many-body systems are at the heart of theoretical physics, with applications extending from celestial mechanics to quantum matter. A particularly important class of these systems is governed by distance-dependent potentials, where the interaction energy between any two particles depends only on the scalar distance between them. These potentials, often symmetric under spatial transformations, give rise to rich symmetry structures that can dramatically simplify the analysis of otherwise complex systems.

Symmetries play a central role in modern physics—not only offering conservation laws via Noether's theorem but also guiding the formulation of solvable models and invariant quantities. Systems with radial potentials, such as gravitational or electrostatic interactions, inherently possess rotational symmetry, while systems with homogeneous pairwise interactions may exhibit translational and scaling symmetries.

In this work, we focus on the implications of distance-based interaction functions in multi-particle systems. We analyze the conserved quantities associated with continuous symmetries (e.g., angular momentum for rotational invariance), identify conditions for integrability, and investigate how perturbations in the potential form influence symmetry breaking. Through both analytical approaches and theoretical modeling, this study builds a deeper understanding of the relationship between potential form and symmetry conservation in physical systems.

The configuration of a system of N atoms at positions qi , i = 1, 2, . . . , N, is defined as a 3N-dimensional vector q = (q1, q2, . . . , qN) ∈ R 3N . We note that these can provisionally be thought of as vertices of an N-gon, or an N-polyhedron, assuming that qi 6= qj for i 6= j. The lengths of edges are distances between atoms, which we denote by

$$r_{ij} = |\mathbf{q}_j - \mathbf{q}_i|, \quad \text{for} \quad i, j = 1, 2, \ldots, N. \qquad (1)$$

In this paper, we study potential functions U : R 3N → R called central potential functions which satisfy certainsymmetries as specified in Definition 1. These symmetries are: (i) translational invariance; (ii) rotational invariance; (iii) reflectional invariance; and (iv) parity for i,j identical atoms. An example of potential satisfying the assumptions in Definition 1 is

$$U(\mathbf{q}) = \sum_{i<j}^{N} \Psi_2(r_{ij}) + \sum_{i<j<k}^{N} \Psi_3(r_{ij}, r_{ik}, r_{jk}), \qquad (2)$$

The symmetries considered in Definition 1 are satisfied by other generalizations of the example potential (2), which include n-body terms depending only on the distances (1) between atoms. In fact, the symmetries (i)-(iv) imply that the potential U : R 3N → R can be written as a function of distances. We have the following theorem which we prove in Section III.

Theorem 1. A central potential function U : R 3N −→ R can be written as

$$\phi : [0, \infty)^{N(N-1)/2} \to \mathbb{R},$$

where the N(N − 1)/2 inputs are interpreted as the set of all pairwise distances (1) between atoms. Considering N = 2, Theorem 1 states that a central potential function U of 6 variables can be written as a function φ of 1 variable, r12. Consequently, Theorem 1 reduces the dimensionality of the potential U for any N < 7. If N = 7, then we have 3N = N(N − 1)/2 = 21 and the 21-dimensional state space R 3N corresponds to the 21 distance variables (1). Since the dimension of the state space scales as O(N) and the number of distances scales as O(N2), Theorem 1 can be further improved by considering only a subset of the distance variables (1). In Section III, we also prove the following result.

Theorem 2. Let N ≥ 4. Then a central potential function U : R 3N −→ R can be written as

$$\phi : [0, \infty)^{4N-10} \to \mathbb{R},$$

where the (4N − 10) inputs are a subset of the set of all pairwise distances (1). Considering N = 4 and N = 5, we have 4N −10 = 6 and 4N − 10 = 10, respectively. In particular, Theorems 1 and 2 state the same conclusion for N = 4 and N = 5. Theorem 2 improves the result of Theorem 1 for N > 5. We will prove Theorems 1 and 2 together in Section III by considering the cases N = 2, N = 3, N = 4, N = 5 and N > 5. Applying Theorem 2 to our example potential (2), we observes that it reduces the number of independent variables for N > 5. In particular, while function φ constructed in the proof of Theorem 2 depends only on distances (1), it is not given in the form (2). In addition to central potential functions satisfying conditions in Definition 1, there are potentials to which Theorems 1 and 2 are not applicable. For example, if the potential U corresponds to an external non-uniform

$$U(\mathbf{q}) = \sum_{i=1}^{N} \Psi_1(\mathbf{q}_i)$$

and U will neither satisfy the conditions in Definition 1, nor will it be possible to write as a function of pairwise distances (1). Assuming that there is no external field present and that we have a system of N identical atoms interacting (i.e. U satisfies condition (iv) in Definition 1), then we can formally write it as a sum of the n-body interactions for 2 ≤ n ≤ N in the form

$$U(\mathbf{q}) = \sum_{i<j}^{N} U_2(\mathbf{q}_i, \mathbf{q}_j) + \sum_{i<j<k}^{N} U_3(\mathbf{q}_i, \mathbf{q}_j, \mathbf{q}_k) + \dots$$
$$\dots + U_N(\mathbf{q}_1, \dots, \mathbf{q}_N), \quad (3)$$

where we can naturally think about n-polyhedrons of atoms as the input to the potential function, but these are fixed in space and a natural assumption is that given this input, it should not matter where we fix this polyhedron (leading to translational invariance (i)), or how we orient this polyhedron (rotational invariance (ii)). One slightly more subtle assumption, is that we should be allowed to reflect our polyhedron in any plane that keeps the polyhedron on one side (reflectional symmetry (iii)). One difference between symmetries (i)–(ii) and (iii)– (iv) is that the former ones are continuous symmetries whereas the reflection invariance (iii) and parity (iv) are not. Noether's theorem [27] states that each continuous symmetry gives rise to a corresponding conserved quantity (in a closed system). In particular, translational invariance (i) leads to conserved linear momentum (which is a consequence of reciprocity of forces) and rotational invariance (ii) gives rise to conserved angular momentum. In the next section, we provide a proof that functions obeying symmetries (i)–(iv) should only rely on distances and we also show that a proper subset of pairwise distances for N > 5 can be used to describe the potential function U.

II. PROOFS OF THEOREMS 1 AND 2

We prove Theorems 1 and 2 together by considering the cases N = 2, N = 3, N = 4 and N = 5, followed by an inductive argument for N > 5. We define displacement vectors by

$$\boldsymbol{\Delta}_{ij} = \mathbf{q}_j - \mathbf{q}_i, \quad \text{for} \quad i, j = 1, 2, \ldots, N, \qquad (4)$$

i.e. we have $r_{ij} = |\boldsymbol{\Delta}_{ij}|$.

A. The case N = 2

We define function φ : [0,∞) → R by

$$\phi(s) = U(\mathbf{0}, s\hat{\mathbf{k}}) = U(0, 0, 0, 0, 0, s), \qquad (5)$$

where kˆ is a unit vector in the direction of the positive z axis and 0 = [0, 0, 0]. Given atom positions q1, q2 ∈ R 3 , we translate the configuration to position atom 1 at the origin. Using symmetry (i) in Definition 1, we have U(q1, q2) = U(0, Δ12). We then rotate the axes using rotation R1 ∈SO(3) such that the displacement vector connecting the two atoms is aligned with the positive z axis, giving R1Δ12 = r12kˆ, while maintaining R10 = 0. Using symmetry (ii) in Definition 1, we have

$$U(\mathbf{q}_1, \mathbf{q}_2) = U(\mathbf{0}, \boldsymbol{\Delta}_{12}) = U(\mathbf{0}, r_{12}\hat{\mathbf{k}}) = \phi(r_{12}),$$

where the last equality follows from our definition (5). This concludes the proof of Theorem 1 for N = 2.

B. The case N = 3

Given atom positions q1, q2, q3 ∈ R 3 , we consider the function U(q1, q2, q3). Using symmetry (i) in Definition 1, we translate the configuration to position atom 1 at the origin and consequently, we have

$$U(\mathbf{q}_1, \mathbf{q}_2, \mathbf{q}_3) = U(\mathbf{0}, \boldsymbol{\Delta}_{12}, \boldsymbol{\Delta}_{13}).$$

Given that we have three axes to rotate around, we canalways find a rotation R1 such that R1Δ12 = r12kˆ, as wedid in the N = 2 case. Using symmetry (ii), we have

$$U(\mathbf{q}_1, \mathbf{q}_2, \mathbf{q}_3) = U(\mathbf{0}, r_{12}\hat{\mathbf{k}}, R_2R_1\boldsymbol{\Delta}_{13}).$$

However the key point is that R2R1Δ13 is uniquely defined by the triangle with lengths r12, r13 and r23, theangles of which can be calculated using the cosine rule,i.e. R2R1Δ13 can be expressed as

$$\left[\sqrt{r_{13}^2 - \left(\frac{r_{13}^2 + r_{12}^2 - r_{23}^2}{2r_{12}}\right)^2}, 0, \frac{r_{13}^2 + r_{12}^2 - r_{23}^2}{2r_{12}}\right]. \qquad (6)$$

Therefore there exists function φ : [0,∞)3 → R suchthat U(q1, q2, q3) = φ(r12, r13, r23), for any q1, q2 andq3, confirming Theorem 1 for N = 3.

C. The case N = 4

Given atom positions q1, q2, q3, q4 ∈ R3, these can bethought of defining the vertices of a tetrahedron (or ifco-planar a quadrilateral). Following similar steps as inthe case N = 3 in Section III B, we translate atom 1

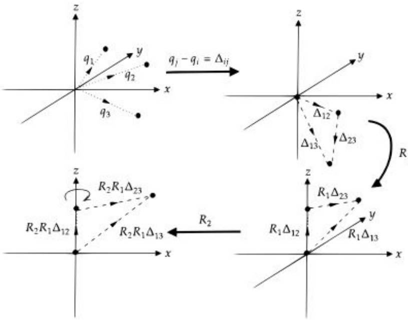

FIG. 1. A schematic of the constructive method in aid of theproof for the case N = 3.to the origin, apply rotation R1 to orient displacementvector Δ12 with the positive z axis, then do a secondrotation R2 that fixes the triangle formed by the verticesof atoms 1, 2 and 3 in the x-z plane. As in Section III B,we have

Using equation (6), we know that R2R1Δ13 is determined entirely by distances r12, r13 and r23. All thatremains to be shown is that R2R1Δ14 is determined bypairwise istances. We note that the triangle formed byatoms 1, 2 and 3 (denoted as ABC in the lower partof our illustration of the proof in Figure 2) is uniquelydetermined (after orienting one side with the positive zaxis). Consequently, this fixes the side BC. On the otherhand the triangle BCD is uniquely determined (as oneside BC is fixed) by distances r23, r24 and r34. These canbe thought of as two triangles which can rotate around ahinge BC, so to determine the vector R2R1Δ14, we necessarily need the final distance r14 that gives the anglebetween the planes containing triangles ABC and BCD(two configurations are illustrated in Figure 2). If triangles ABC and BCD are co-planar, the set of all pairwise distances, with this orientation, will give a uniquedescription of R2R1Δ14. If these triangles are not coplanar, this final distance gives two possible vectors forR2R1Δ14. These correspond to a unique R2R1Δ14 andthe copy obtained by reflection in the plane containingtriangle ABC. However by property (iii) we know thatif we reflect in the plane containing ABC with a matrixdenoted Q, then

IV. CONCLUSIONS

This study has explored how symmetry principles emerge and are conserved in multi-particle systems governed by distance-dependent interaction potentials. We have shown that such systems often exhibit rotational, translational, and sometimes scaling symmetry, depending on the specific form of the potential function. These symmetries lead to conserved quantities such as angular momentum and total linear momentum, which play vital roles in understanding both the qualitative and quantitative behavior of the system.

Importantly, we demonstrated that the invariance of the potential under certain transformations directly determines the dynamical symmetries and integrability of the many-body model. When such symmetry conditions are slightly violated—through external fields, anisotropic modifications, or time dependence—the corresponding conservation laws are broken, leading to more complex, often chaotic behavior.

In conclusion, distance-dependent interactions serve as a foundation for exploring symmetry-driven dynamics in many-body physics. The findings provide a framework for future studies in quantum many-body systems, molecular dynamics, and gravitational models, where symmetry continues to offer a guiding principle in the search for analytical solutions and physical insights.

REFERENCES

[1] J. Murrell et al. Molecular potential energy functions. Wiley (1984)

[2] G. Ackland. Interatomic potential development. Comprehensive Nuclear Materials, pp. 267-291 (2012)

[3] W. Noid. Perspective: coarse-grained models for biomolecular systems. Journal of Chemical Physics 139(9), 090901 (2013)

[4] M. Hoef and P. Madden. Three-body dispersion contributions to the thermodynamic properties and effective pair interactions in liquid argon. Journal of Chemical Physics 111(4), pp. 1520-1526 (1999)

[5] A Louis. Beware of density dependent pair potentials. Journal of Physics: Condensed Matter 14, pp. 9187 (2002)

[6] M. Sprik Effective pair potentials and beyond. In: Computer Simulation in Chemical Physics. NATO ASI Series, vol 397, Springer, Dordrecht (1993)

[7] C. Zhao et al. Seven-site effective pair potential for simulating liquid water. Journal of Physical Chemistry B 123(21), pp. 4594–4603 (2019)

[8] J. Bomont and J. Bretonnet. An effective pair potential for thermodynamics and structural properties of liquid mercury. Journal of Chemical Physics 124, 054504 (2006)

[9] J. Utterson and R. Erban. On standardised moments of force distribution in simple liquids. Physical Chemistry Chemical Physics 24, pp. 5646-5657 (2022)

[10] K.O. Waseda. Structure and effective pair potential of liquid silicon. Japanese Journal of Applied Physics 35, pp. 151 (1996)

[11] R. Erban and S.J. Chapman. Stochastic modelling of reaction-diffusion processes. Cambridge Texts in Applied Mathematics, Cambridge University Press (2020) 7

[12] S. Plimpton and A. Thompson. Computational aspects of many-body potentials. MRS Bulletin. Cambridge University Press 37(5), pp. 513–521 (2012)

[13] G. Cisneros et al. Modeling molecular interactions in water: from pairwise to many-body potential energy functions. Chemical Reviews 116(13), pp. 7501–7528 (2016)

[14] F. Stillinger and T. Weber. Computer simulation of local order in condensed phases of silicon. Physical Review B 31(8), pp. 5262 (1985)

[15] R. Biswas and D. Hamann. New classical models for silicon structural energies. Physical Review B 36(12), pp. 6434 (1987)

[16] M. Daw and M. Baskes. Embedded-atom method: Derivation and application to impurities, surfaces, and other defects in metals. Physical Review B 29(12), pp. 6443 (1984)

[17] R. Richard, K. Lao and J. Herbert. Understanding the many-body expansion for large systems. I. precision considerations. Journal of Chemical Physics 141(1), 014108 (2014)

[18] J. Sanchez, F. Ducastelle and D. Gratias. Generalized cluster description of multicomponent systems. Physica A: Statistical Mechanics and its Applications 128(1-2), pp. 334-350 (1984)

[19] R. Drautz, M. F¨ahnle, and J. Sanchez. General relations between many-body potentials and cluster expansions in multicomponent systems. Journal of Physics: Condensed Matter 16(23), pp. 3843 (2004)

[20] S. Loos et al. Nonreciprocal forces enable cold-to-hot heat transfer between nanoparticles. Scientific Reports 13, 4517 (2023)