THE WIGNER–ECKART THEOREM FOR REDUCIBLE SYMMETRIC CARTESIAN TENSOR OPERATORS

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We explicitly establish a unitary correspondence between spherical irreducible tensor operators and Cartesian tensor operators of any rank. That unitary relation is implemented by means of a basis of integer-spin wave functions that constitute simultaneously a basis of the spaces of Cartesian and spherical irreducible tensors. As a consequence, we extend the Wigner–Eckart theorem to Cartesian irreducible tensor operators of any rank, and to totally symmetric reducible ones. We also discuss the tensorial structure of several standard spherical irreducible tensors such as ordinary, bipolar and tensor spherical harmonics, spin-polarization operators and multipole operators. As an application, we obtain an explicit expression for the derivatives of any order of spherical harmonics in terms of tensor spherical harmonics.

Keywords: spherical tensor, Cartesian tensor, spherical harmonic, angular momentum, Wigner–Eckart theorem.

1. Introduction

The Wigner–Eckart theorem is one of the fundamental results in quantum angular-momentum theory. As is well known, it states that the dependence on magnetic quantum numbers of the matrix elements of spherical irreducible tensor operators (henceforth SITOs) between angular–momentum eigenstates, is factorizable into a Clebsch–Gordan (henceforth CG) coefficient. This leads to a drastic simplification of the calculation of tensor-operator matrix elements, such as those appearing in perturbative computations in molecular, atomic and nuclear systems (and more generally in rotationally invariant many-body problems), and a vast array of other quantum-mechanical systems such as, e.g. the theory of anisotropic liquids [1]. By now standard textbook material, the Wigner–Eckart theorem was first formulated by Eckart [2] for rank-1 SITOs and generalized by Wigner [3] to SITOs of any rank. Wigner's treatment is based on group–theoretic methods involving finite rotation operators. The definition of SITOs and the proof of the Wigner–Eckart theorem based on angular-momentum commutation relations (i.e. on infinitesimal rotation operators), as usually found in textbooks [4–7], is due to Racah [8].[1]

[1] A more detailed historical account is given in [9].

In this paper we consider the relationship between SITOs and Cartesian irreducible tensor operators (henceforth CITOs). We explicitly establish a unitary correspondence between them valid for any rank. The precise relation between spherical and Cartesian tensors allows us to apply the technical machinery of tensor algebra to spherical tensors and, conversely, the techniques of quantum angular–momentum theory to Cartesian tensors. That interplay is, in fact, the main subject of this paper. In this respect, our results are a significant extension of the classic work of Zemach [10] and complementary to more recent results (e.g. [11] and references cited there).

Another important feature of our approach is that the coefficients of the unitary transformation relating SITOs and CITOs have a well-defined physical meaning: they are an orthonormal, complete set of standard spin wave functions, satisfying the eigenvalue equations, phase conventions and complex–conjugation properties expected of angular–momentum eigenstates and eigenfunctions which, furthermore, form a Clebsch–Gordan series of angular–momentum states. They transform under rotations either as Cartesian or as spherical tensors, which explains their role in relating both types of tensors. By means of the relation between spherical and Cartesian irreducible tensor operators we extend the Wigner–Eckart theorem to CITOs of any rank. Remarkably, such an extension has not been considered before in the literature. We discuss also the Cartesian tensorial form of several commonly occurring SITOs (ordinary spherical harmonics, as well as bipolar and tensor ones, among others). Those Cartesian expressions provide a viewpoint complementary to the usual analytical one, by making the tensorial structure of SITOs completely explicit, which makes possible to obtain relations that would otherwise be more difficult to find. Furthermore, writing SITOs in tensorial form is of interest in the context of relativistic theories, for example in connection with covariant partial-wave expansions. The converse case is also true, since by mapping Cartesian tensors into spherical ones their angular–momentum properties become apparent.

Reducible Cartesian tensors occur frequently in physics, so the evaluation of the angular-momentum matrix elements of reducible tensor operators is clearly of interest. We obtain in this paper a further extension of the Wigner–Eckart theorem to a limited class of reducible tensor operators of any rank, namely, that of totally symmetric ones. This allows us to compute the matrix elements of tensor powers of the position and of the momentum operators. As an application, we obtain an explicit expression for the gradients of spherical harmonics to all orders in terms of tensor spherical harmonics. That result is a generalization of the well-known gradient formula [7, 12, 13] for first derivatives to derivatives of any order.

The paper is organized as follows. In the following section we introduce the spin operator for Cartesian tensors and briefly discuss our notation and conventions for tensors. In Section 3 we construct a standard basis of spin wave functions for any integer spin and establish their main properties both as angular–momentum eigenfunctions and as a basis of the space of Cartesian irreducible tensors. By means of that basis, in Section 4 we obtain the unitary relation between SITOs and CITOs. In Section 5 we establish the Wigner–Eckart theorem for CITOs. In Section 6 we analyze several SITOs commonly used in the literature, including