On irreducible spherical tensor operators and “modern” textbooks on quantum mechanics: the perpetuation of nonsense.

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Despite its title, this note does not attempt a case study nor a serious sociological, or philosphical discussion (c.f. [2]). It just presents an instance of a phenomenon which the title attempts to describe; specifically how two modern textbooks present the subject ‘irreducible spherical tensor operators’ in quantum theory. It was written for the students taking the 2014 edition of the lectures in Quantum Mechanics at the Facultad de Matemática, Astronomía y Física of the national university in Córdoba, Argentina; and, with minor expectations, for some of my colleagues. To inform the reader on my perspective, I must say that upon returning to the teaching of quantum mechanics after spending roughly ten years teaching other subjects in our physics curricula, I found a certain ‘modernization’ had taken place. This was, for example, apparent in the excercises where I detected a persistent presence of notations and formulations used by texts such as the well-known books by Ballentine [1] or that by Zettili [8]. I must also confess that I hadn’t read these texts at all. If sorely pressed by some serious student who asks me to recommend a quantum mechanics textbook, my answer is, invariably, the book by Albert Messiah, [4], the preface of which is dated October, 1958. After my lectures on irreducible spherical tensor operators (I will shorten this to ISTO’s) a student, Natalia Giovenale, informed me that my story was in blatant contradiction with Zettili’s presentation. So I had to do my chores and here is what I saw.
In Ballentine’s book ISTO’s are presented in section 7.8 beginning on page 193; there you are informed that a set of $2k+1$ operators $\{T_q^{(k)} : (-k \leq q \leq k)\}$ form an *irreducible tensor of degree* k[1] if

$$\boldsymbol{R}(\alpha,\beta,\gamma)T_q^{(k)}\boldsymbol{R}^{-1}(\alpha,\beta,\gamma) = \sum_{q'} T_{q'}^{(k)} D_{q',q}^{(k)}(\alpha,\beta,\gamma)\ . \tag{1}$$

This is eq. (7.108) of Ballentine and is Wigner’s original definition [7]. With apologies to the knowledgeable, the various symbols stand for the following. (α,β,γ) are the Euler angles for a rotation in real three dimensional euclidean space around a direction $\widehat{\boldsymbol{n}}$ (in $\mathbb{R}^3$ with unit length) by an angle ϕ, say with the usual convention regarding the sign of ϕ and the sense of rotation.

$$\boldsymbol{R}(\alpha,\beta,\gamma) = \exp\{-i\phi\widehat{\boldsymbol{n}}\cdot\boldsymbol{J}/\hbar\}\ , \tag{2}$$

[1] The qualifier ‘spherical’ is not used which is perfectly allright although I will continue to insist with the acronym ISTO.

where the angular momentum operator-triple $\boldsymbol{J} = (J_1, J_2, J_3)$ consists of self-adjoint operators acting on a Hilbert space and satisfying the commutation relation $[J_1, J_2] = i\hbar J_3$ and the other two obtained form this one by cyclic permutation of the indices $\{1, 2, 3\}$[2]. The $(2k+1)\times(2k+1)$ matrix $D(\cdots)$ whose matrix elements (in an orthonormal basis to be specified shortly) enter in the right-hand side of Wigner's defining equation (1) is

$$D(\alpha, \beta, \gamma) = \exp\{-i\phi\widehat{\boldsymbol{n}} \cdot \boldsymbol{S}^{[k]}/\hbar\} \; , \tag{3}$$

where the angular momentum $\boldsymbol{S}^{[k]}$ is an irreducible angular momentum of magnitude k; that is to say it is an angular momentum $\boldsymbol{S}$ acting on a Hilbert space (say $\mathcal{K}$) in such a way that $[A, S_j] = 0$ for $j = 1, 2, 3$ and for an operator A on $\mathcal{K}$ implies that A is a multiple of the identity[3]. It follows, because $\boldsymbol{S}^2$ always[4] commutes with each component of $\boldsymbol{S}$ that $\boldsymbol{S}^2 = \hbar^2 k(k+1)\mathbf{1}$ where k is some integer multiple of $1/2$, and the dimension of $\mathcal{K}$ is $2k+1$. Moreover, two such irreducible angular momenta for the same k are necessarily unitarily equivalent (there is an unitary U such that $\mathcal{K}' = U\mathcal{K}$ and $\boldsymbol{S}'U = U\boldsymbol{S}$); this is the reason for the superscript $[k]$. And, finally, for any $k \in \{0, 1/2, 1, 3/2, \cdots\}$ there is such an irreducible angular momentum –now called $\boldsymbol{S}^{[k]}$– acting on a Hilbert space of dimension $(2k+1)$ conveniently denoted by $\mathfrak{H}^{[k]}$. The story continues as follows: given $\boldsymbol{S}^{[k]}$ the spectrum of each of its three components is $\{\hbar q : q \in \{-k, -k+1, -k+2, \cdots, k\}\}$ so that each eigenvalues is simple (i.e., non-degenerate). There then is, of course, an orthonormal basis $\{|k, q\rangle : q \in \{-k, -k+1, -k+2, \cdots, k\}\}$ which diagonalizes the third component $S_3^{[k]}$ but, again due to the angular momentum commutation relations, can also be forced to satisfy $S_\pm^{[k]}|k, q\rangle = \hbar\sqrt{k(k+1) - q(q\pm 1)}\;|k, q\pm 1\rangle$. Such a basis –I will refer to a standard-basis– is unique (!) up to multiplication of all the basis elements by one and the same complex constant of modulus 1; in particular the matrix-elements, i.e. the numbers $D^{(k)}_{q'q}(\alpha, \beta, \gamma)$, are uniquely specified by the single parameter k along with the Euler angles.

Thus, (1) states that an ISTO is a collection of $2k+1$ operators that transform with respect to rotations (generated by some angular momentum namely $\boldsymbol{J}$) as do the $2k+1$ elements of a standard basis of $\mathbb{C}^{2k+1}$ upon a 'rotation' in this latter space.
Proceeding from (1) the text of Ballentine continues and claims that this equation may be rewritten as (omitting the Euler angles)[5]:

$$\boldsymbol{R}T^{(k)}_q\boldsymbol{R}^{-1} = \sum_{q'} T^{(k)}_{q'}\langle k, q'|\boldsymbol{R}|k, q\rangle \; ; \tag{4}$$

and this claim is simply wrong because the rotation matrix $D^{(k)}$ is confused with the matrix associated with the rotation (operator) $\boldsymbol{R}$! To show that the right-hand side of (4) is meaningless, consider a pure spin 1/2, so that in my notation $\boldsymbol{J} = \boldsymbol{S}^{[1/2]}$. The operator $\boldsymbol{J}$ is a vector operator with respect to itself so that transforming into spherical components

$$T^{(1)}_o := J_3 \; , \;\; T^{(1)}_{\pm 1} := \mp(J_1 \pm iJ_2)/\sqrt{2} \; ,$$

[2]Frequently and interestingly the components of the angular momentum are unbounded and this necessitates the addition of sufficient salt and pepper in the form of domain questions in order to become mathematically digestible. In a textbook one sticks to the algebraic aspects only which are really the crucial ones.

[3]Alternatively, Schur's Lemma states that this is equivalent to demanding that the only subspaces of $\mathcal{K}$ which are invariant under all $\boldsymbol{R}'s$ are the trivial ones $\mathcal{K}$ and 0.

[4]Due to the angular momentum commutation relations.

[5]The eq. is unnumbered in Ballentine (foot of p.193)

$T_q^{(1)}$ $(q = 1, 0, -1)$ is certainly an ISTO of degree 1 with respect to $\boldsymbol{J}$. However, the r.h.s of (4) asks us (in order to verify the defining identity) to compute $3 \times 3 = 9$ matrix-elements of an operator acting in a 2-dimensional Hilbert space ! The correct version of the culprit is of course, with (3):

$$\boldsymbol{R} T_q^{(k)} \boldsymbol{R}^{-1} = \sum_{q'} T_{q'}^{(k)} \langle k, q' | D^{(k)} | k, q \rangle \; ; \tag{5}$$

where, to insist again

$$\boldsymbol{R}(\alpha, \beta, \gamma) = e^{-i\phi \widehat{\boldsymbol{n}} \cdot \boldsymbol{J}/\hbar} \; , \;\; D^{(k)}(\alpha, \beta, \gamma) = e^{-i\phi \, \widehat{\boldsymbol{n}} \cdot \boldsymbol{S}^{[k]}/\hbar} \; ;$$

$\boldsymbol{R}$ acts on wherever the reference angular momentum $\boldsymbol{J}$ is defined whereas $D^{[k]}$ acts in the $(2k+1)$-dimensional Hilbert space $\mathfrak{H}^{[k]}$ where the irreducible elementary spin of magnitude k is defined.
The error incurred propagates; the infinitesimal version of (4) is then Ballentine's eq. (7.111)

$$[\widehat{\boldsymbol{n}} \cdot \boldsymbol{J}, T_q^{(k)}] = \sum_{q'} T_{q'}^{(k)} \langle k, q' | \widehat{\boldsymbol{n}} \cdot \boldsymbol{J} | k, q \rangle \tag{6}$$

where, concomitantly, the r.h.s is meaningless because $\widehat{\boldsymbol{n}} \cdot \boldsymbol{J}$ acts on the Hilbert space carrying $\boldsymbol{J}$ and $\{|k, q\rangle\}$ is the same good, old, orthonormal basis of $\mathfrak{H}^{[k]} \equiv \mathbb{C}^{2k+1}$. Of course, differentiating (5) –with (2) and (3) in mind– with respect to the rotation-angle ϕ and setting $\phi = 0$– we get the correct version, due to Racah,

$$[\widehat{\boldsymbol{n}} \cdot \boldsymbol{J}, T_q^{(k)}] = \sum_{q'} T_{q'}^{(k)} \langle k, q' | \widehat{\boldsymbol{n}} \cdot \boldsymbol{S}^{[k]} | k, q \rangle \; . \tag{7}$$

By an irreproducible tour de force starting from (6), Ballentine lands atop his equations (7.112a,b,c) which is the usual -and perfectly correct infinitesimal version of the definition of an ISTO due to Racah [5]:

$$[J_3, T_q^{(k)}] = \hbar q T_q^{(k)} \; , \;\; [J_\pm, T_q^{(k)}] = \hbar \sqrt{k(k+1) - q(q \pm 1)} T_{q\pm1}^{(k)} \; . \tag{8}$$

This follows from (7) by choosing $\widehat{\boldsymbol{n}}$ to be first, the unit vector in the z or third direction and then to be the spherical vectors $\widehat{\boldsymbol{n}}_\pm := (\widehat{\boldsymbol{x}} \pm i \widehat{\boldsymbol{y}})/\sqrt{2}$. It is also obviously equivalent to (7) because these three vectors are just another linearly independent system in $\mathbb{C}^3$. Supposedly, the same procedure involving the meaningless formulae

$$\langle k, q' | J_3 | k, q \rangle = \hbar q \; \delta_{q',q} \; , \;\; \langle k, q' | J_\pm | k, q \rangle = \hbar \sqrt{k(k+1) - q(q \pm 1)} \delta_{q',q\pm1}$$

lead from nonsensical (6) to the correct eq. (8). Notice that the presence and crucial role of the second angular momentum $\boldsymbol{S}^{[k]}$ is entirely hidden but encoded in the numerical factors on the r.h.s of Racah's equation (8). Ballentine then continues to digress on ISTO's arriving eventually to the Wigner-Eckart Theorem of which a (correct) proof is given. I am not at all prepared to follow through each and every claim or calculation performed after or using the meaningless unnumbered equation (4) and its alter ego (7.111). As far as I was willing to check, the rest of the formulas of 7.8 are correct.

Something entirely similar ocurrs in Zettili's book. Although the (integrated, global and extremely useful) versions (1) and the false (4) are not presented at all as far as I see, the infamous (6) appears in various guises as eqs. (7.309) all the way up to (7.314) and, then (7.317); all of them nonsensical.

The book by Leslie E. Ballentine's first edition is claimed in the preface to be from 1990 (Prentice-Hall) although the World-Scientific edition is from 1998, with various reprints (the copy I examined is from 2001). The book by Nouredine Zettili is a publication of 2001; in its preface it claims to be, basically, a problem solving book, and Ballentine's book is cited. Is there something special about these two specific books mentioned here? Do both have some common ancestor? Have they been reviewed in the relevant physics journals? Why have these (and other) mistakes not been corrected? What about other "modern" books on quantum mechanics? I do not know and I am not willing to lose much time in finding out. But both are sold for good money on the recommendation of learned professors to young people eager to discover the subtleties of quantum theory.

I certainly do not see any reason whatsoever to replace my Dover edition of Messiah (two volumes bound as one) by anything more modern[6]. And I plea: stop this propagation of nonsense.

References

[1] Ballentine, L.E.: Quantum Mechanics. A Modern Development. World Scientific, Singapore 1998.

[2] Frankfurt, H. G.: On Bullshit, Princeton University Press, Princeton 2005.

[3] Galindo, A. and Pascual, P. : Quantum Mechanics, Vol. 1 & 2., Springer-Verlag, Berlin, 1990 and 1991.

[4] Messiah, A.: Mécanique Quantique, Tome I & II. Dunod, Paris 1960. English translation as 'Quantum Mechanics' published 1961-1962 by North-Holland, New York.

[5] Racah, G.: Phys. Rev. **61**, 186 (1942); Phys. Rev. **62**, 438 (1942); Phys. Rev. **63**, 467 (1942).

[6] Straumann, N.: Quantenmechanik. Nichtrelativistische Quantentheorie. Springer-Verlag, Berlin 2002.

[7] Wigner, E.: Gruppentheorie und ihre Anwendung auf die Quantenmechanik der Atomspektren, Vieweg und Sohn, Braunschweig, 1931. English translation as 'Group Theory and Its Application to the Quantum Mechanics of Atomic Spectra' published by Academic Press, New York, in 1959.

[8] Zettili, N.: Quantum Mechanics. Concepts and Aplications. J. Wiley & Sons, Chichester 2001.

[6] Alongside, I also keep Norbert Straumann's "Quantenmechanik" [6] which I gauge as a both modern and excellent (advanced) textbook and the two volumes by Galindo and Pascual [3] which although not a textbook, is a reliable and wonderful Pandora's box.