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A Tensorial Formalism for Studying Orbital and Spin States in a Multielectron System

M.A. Grado-Caffaro and M. Grado-Caffaro

Scientific Consultants, C/Julio Palacios 11, 9-B, 28029-Madrid, Spain

Abstract

We present a tensorial formalism to investigate the physics of a given multielectron system from the standpoint of orbital and spin states. In fact, we determine the space of total quantum states as tensor product between the space of orbital states and the space of spin states. This product is the usual tensor product in the Krönecker sense employed in Quantum Mechanics but, in our formalism, we employ also a different tensor product which we call dyadic-tensorial product.

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1. Introduction

In all branches of Physics, matrix formulations are certainly elegant and also very useful. Unfortunately, some people (obviously, without solid mathematical background) "believe" that the above formulations are, say, unuseful manipulations. Really, this "belief" is inadmissible. In both Mathematical Physics and Theoretical Physics, matrix formalisms are necessary. These formalisms can be based, currently, on tensor or dyadic products. On the other hand, multielectron systems play a significant role in several areas of Physics and Chemistry. In this context, let us consider multielectron atoms or Fermi gases. Indeed, the physics of fermionic gases is an important subject which, to date, has been investigated extensively. Nevertheless, a number of questions remain open upon the above subject and related issues [1-4] as, for example, density of states.

In the following, we shall perform a mathematical analysis on atomic-orbital and spin states in a given multielectron system. As a matter of fact, we shall establish a relatively abstract matrix-tensor formalism to study accurately the aforementioned system. But that our formalism be somewhat, say, abstract does not imply that it be unuseful (regard the beginning of this section). We will employ the concept of standard tensorial product in Quantum Mechanics and also a dyadic-tensor product [5-8] distinct from the above product. With these ingredients, an elegant and accurate formulation will be derived.

2. Theory

Given a certain multielectron system, under a time-independent framework, we start from the following expression:

$$T = \Omega \otimes S \tag{1}$$

where T is the total space (Hilbert) of quantum states in the system, Ω is the atomic-orbital space, and S is the spin space. In addition, we have that $S = S^{(u)} \oplus S^{(d)}$ where $S^{(u)}$ and $S^{(d)}$ denote, respectively, spin-up space and spin-down space, respectively. Inserting this last expression into formula (1), the total space of quantum states splits into two parts (as direct sum of them) as follows:

$$T^{(u)} = \Omega \otimes S^{(u)} \tag{2}$$

$$T^{(d)} = \Omega \otimes S^{d} \tag{3}$$

On the other side, a generic atomic-orbital (electron) wavefunction relative to a basis $\{\psi_i\}_1^\infty$ reads:

$$\psi = \sum_i \alpha_i \psi_i \tag{4}$$

where, as we have said, $\psi \in \Omega$.

Furthermore, a generic spin wavefunction relative to a basis $\{\phi_j\}_1^\infty$ is:

$$\phi = \sum_j \beta_j \phi_j \tag{5}$$

where, as we have said, $\phi \in S$.

By combining formulas (1), (4) and (5), one gets for $\psi \otimes \phi \in T$:

$$\psi \otimes \phi = \sum_{i,j} \alpha_i \beta_j \left(\psi_i \otimes \phi_j \right) \tag{6}$$

We want to remark that, of course, the above wavefunctions depend upon spatial coordinates but, for the sake of brevity, the arguments of these functions are omitted. On the other hand, putting $\alpha_i \beta_j \equiv \gamma_{ij}$, relationship (6) becomes:

$$\psi \otimes \phi = tr\left(\Gamma \,\tilde{\otimes}\, G\right) \tag{7}$$

where $\tilde{\otimes}$ denotes the mentioned-above dyadic-tensor product [5-8], *tr* designates trace, and Γ, G are the matrices $\Gamma = \left(\gamma_{ij}\right)$, $G = \left(g_{ij}\right)$ with $g_{ij} = \psi_i \otimes \phi_j$.

On the other side, we can write:

$$\phi_j = \phi_j^{(u)} + \phi_j^{(d)} \tag{8}$$

Since $g_{ij} = \psi_i \otimes \phi_j$ and by relation (8), it follows:

$$g_{ij} = \left(\psi_i \otimes \phi_j^{(u)}\right) + \left(\psi_i \otimes \phi_j^{(d)}\right) \tag{9}$$

With the above nomenclature, formula (9) reduces to:

$$g_{ij} = g_{ij}^{(u)} + g_{ij}^{(d)} \tag{10}$$

where the first (second) term on the right-hand side of (10) equals the first (second) term on the right-hand side of (9).

3. Conclusions

We have presented a mathematical-physics study in which two tensor products are utilized: the conventional tensor product of standard Quantum Mechanics and a special dyadic-tensorial product (see relation (7)). With these algebraic tools, we have constructed an interesting scheme that can be extrapolated to situations somewhat different than the issue treated in the present article. In particular, tackling issues relative to density of states in specific electron gases could be feasible by using our formalism.

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