



Galilean covariance and the spin-orbit interaction

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We have used the Pauli-Schrödinger equation in its covariant form, that is, written in the light-cone of a five-dimensional De Sitter space-time. Following standard procedures, the analogue of the Dirac equation is derived, standing for a galilean spin 1/2 particle in the presence of a external field. Some results are important to be mention, such as the expected g-factor, but in a galilean (not Lorentz) context. In addition, considering interaction, the Pauli-Hartree-Fock equation is obtained following in parallel to the ideas used to construct the Dirac-Hartree-Fock equation.

Keywords: Galilean Covariance, Hartree-Fock, Spin-Orbit

I. INTRODUCTION

It is with the work of Wigner of 1939 [1] that begins the systematic study of the unitary representations Poincaré group, resulting in the development unprecedented for physics, and in particular for relativistic quantum mechanics. In this context, it is the symmetries of space-time that essentially define the structure and dynamics of the mechanical system, and each elementary particle is associated with an irreducible representation of Poincaré's group.

In this way the axiomatic ingredients of relativistic quantum field theory are established in a transparent and general manner; thus elegance [2–4].

Despite the progress that follows Wigner's work in understanding Poincaré's group, it is not until the 1950s that a similar study for non-relativistic quantum mechanics begins. In this case, the symmetry structure is established by the invariance of the Schrödinger equation by space and time transformations, which results in Galilei's group.

The unitary representations of a symmetry group are deduced by associating each group element to a unitary operator meeting the group composition rules [5]. More specifically, consider G a symmetry group with elements $a; b; c; \dots$

For each $a \in G$ is associated a unitary operator $U(a)$

defined in a Hilbert space, such that

$$U(a)U(b) = e^{\phi(a,b)}U(a, b).$$

The phase factor $\phi(a, b)$ is a real and continuous function of a and b . If $\phi(a, b) = 0$ we say that the representation is faithful. Otherwise, the representation is said to be projective. In this situation, a vector in Hilbert's space is less than the phase factor.

Inönü and Wigner [6], studying the unitary representations of Galilei's group, concluded that with the reliable representations, it would not be possible to construct localized wave functions that had sharp velocities. That is, such representations should be dismissed as possible candidates to describe a non-relativistic quantum particle. On the other hand, Bargman [7] showed that for the rotation group, Lorentz and Poincaré, projective representations could be reduced to a faithful representation. However, this is not the case with Galilei's group, where projective representations in general are not reducible to faithful representation [8]. In a synthesis of the works of Inönü, Wigner and Bargman, and Hamermesh [9], studying Lie algebra of the Galilei group, was established that the position and momentum operators could be defined only for the case of projective representations, which are now also called physical representations [10]. Since then, interest in unitary representations describing Galilean symmetries has focused mainly, and as with the Poincaré group, on the study of conformal and internal symmetry structures (In this situation, spin variables appear for consistency in non-relativistic physics, not as a property of Lorentzian invariance). [11–18].

It is in this sense that Takahashi [20–22] introduced a covariant version for Galilei's group based on penta-

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dimensional tensors. This method has been used, in particular, to reduce nonlinear field equations, from which the rearrangement of superfluid symmetries has been analyzed in connection with Goldstone bosons. Another aspect of interest is the study of representations describing non-relativistic particles with arbitrary spin. For a more detailed reading [23].

we will present the formalism to arrive at the explicitly covariant form of the Pauli-Schrödinger equation and show some applications of this formalism, such as the development of the Pauli-Hartree-Fock equation (PHF) and the natural appearance of spin-orbit interaction (without the need of perturbation theory) due to the metric chosen, with a similar approach used in literature [25].

II. GALILEAN COVARIANCE

The Galilei transformations are given by

$$\mathbf{x}' = R\mathbf{x} + \mathbf{v}t + \mathbf{a} \quad (1)$$

$$t' = t + b \quad (2)$$

where R stands for the three-dimensional Euclidean rotations, v is the relative velocity defining the Galilean boosts, \mathbf{a} stands for spacial translations and \mathbf{b} , for time translations. Consider a free mass particle m ; the mass shell relation is given by $p^2 - 2mE = 0$.

We can then define a 5-vector, $p^\mu = (p_x, p_y, p_z, m, E) = (p^i, m, E)$, with $i = 1, 2, 3$.

Thus, we can define a scalar product of the type

$$p_\mu p_\nu g^{\mu\nu} = p_i p_i - p_5 p_4 - p_4 p_5 = p^2 - 2mE = k, \quad (3)$$

where $g^{\mu\nu}$ is the metric of the space-time to be construct, e $p_\nu g^{\mu\nu} = p^\mu$.

Let us define a set of canonical coordinates q^μ associated with p^μ , by writing a five-vector in M , $q^\mu = (\mathbf{q}, q^4, q^5)$, \mathbf{q} is the canonical coordinate associated with p ; q^4 is the canonical coordinate associated with E , and thus can be considered as the time coordinate; q^5 is the canonical coordinate associated with m explicitly given in terms of \mathbf{q} and q^4 , $q^\mu q_\mu = q^\mu q^\nu \eta_{\mu\nu} = \mathbf{q}^2 - 2q^4 q^5 = s^2$. From $q^5 = \frac{\mathbf{q}^2}{2t}$; or infinitesimally, we obtain $\delta q^5 = \mathbf{v} \cdot \delta \frac{\mathbf{q}}{2}$. Therefore, the fifth component is basically defined by velocity.

That can be seen as a special case of a scalar product in G denoted as

$$(x|y) = g^{\mu\nu} x_\mu y_\nu = \sum_{i=1}^3 x_i y_i - x_4 y_5 - x_5 y_4, \quad (4)$$

where $x^4 = y^4 = t$, $x^5 = \frac{x^2}{2t}$ e $y^5 = \frac{y^2}{2t}$. Hence, the following the metric can be introduced

$$(g_{\mu\nu}) = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & -1 & 0 \end{pmatrix}. \quad (5)$$

This is the metric of Galilean manifold \mathcal{G} . In the sequence this structure is explored in order to study unitary representations.

III. THE SCHRÖDINGER EQUATION

Consider a vector $q^\mu \in G$ that obeys the set of linear transformations of the type

$$\bar{q}^\mu = G^\mu{}_\nu q^\nu + a^\mu. \quad (6)$$

A particular case of interest of these transformation, given by

$$\bar{q}^i = R_j^i q^j + v^i q^4 + a^i \quad (7)$$

$$\bar{q}^4 = q^4 + a^4 \quad (8)$$

$$\bar{q}^5 = q^5 - (R_j^i q^j) v_i + \frac{1}{2} \mathbf{v}^2 q^4. \quad (9)$$

In the matrix form, the homogeneous transformations are written as

$$G^\mu{}_\nu = \begin{pmatrix} R_1^1 & R_2^1 & R_3^1 & v^1 & 0 \\ R_1^2 & R_2^2 & R_3^2 & v^2 & 0 \\ R_1^3 & R_2^3 & R_3^3 & v^3 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ v_i R_j^i & v_i R_2^i & v_i R_3^i & \frac{\mathbf{v}^2}{2} & 1 \end{pmatrix}. \quad (10)$$

We can write the generators as

$$\begin{aligned} J_i &= \frac{1}{2} \epsilon_{ijk} \widehat{M}_{jk}, & C_i &= \widehat{M}_{4i}, \\ K_i &= \widehat{M}_{5i}, & D &= \widehat{M}_{54}. \end{aligned} \quad (11)$$

Hence, the non-vanishing commutation relations can be rewritten as

$$\begin{aligned} [J_i, J_j] &= i\epsilon_{ijk} J_k, & [J_i, K_j] &= i\epsilon_{ijk} K_k, \\ [J_i, C_j] &= i\epsilon_{ijk} C_k, & [K_i, C_j] &= i\delta_{ij} D + i\epsilon_{ijk} J_k, \\ [D, K_i] &= iK_i, & [C_i, D] &= iC_i, \\ [p_4, D] &= ip_4, & [J_i, p_j] &= i\epsilon_{ijk} p_k, \\ [p_i, K_j] &= i\delta_{ij} p_5, & [p_i, C_j] &= i\delta_{ij} p_4, \\ [p_4, K_i] &= ip_i, & [p_5, C_i] &= ip_i, \\ [D, p_5] &= ip_5, \end{aligned} \quad (12)$$

This relations form a subalgebra of the Lie algebra of Galilei group in the case of $\mathcal{R}^3 \times \mathcal{R}$, considering J_i the generators of rotations K_i and C_i of the pure Galilei transformations, P_μ the spacial and temporal translations and D of the kind temporal dilatation (which we will not discuss here). In fact, we can observe that eqs. (7) and (8) are the Galilei transformations given by eq. (1) and (1), with $x^4 = t$. The eq. *equationreG - 3* is the compatibility condition which represents the embedding

$$\mathcal{I} : \mathbf{A} \rightarrow A = \left(\mathbf{A}, A_4, \frac{\mathbf{A}^2}{2A_4} \right); \quad \mathbf{A} \in \mathcal{E}_3, A \in \mathcal{G}$$

. The commutation of K_i and P_i is naturally non-zero in his context, so P_5 will be related with mass.

The invariants of this algebra in this context are

$$I_1 = p_\mu p^\mu \quad (13)$$

$$I_2 = p_5 \quad (14)$$

Using the Casimir invariants I_1 and I_2 and applying in Ψ , we have:

$$(p^\mu p_\mu - k^2)\Psi = 0, \quad (15)$$

$$p_5\Psi = -m\Psi \quad (16)$$

where k is an arbitrary constant e $(p^\mu) = (p, p^4, p^5) = p'$, and c' is a velocity constant, and we will take as the unit $c' = 1$. The equation is built on the Galilei manifold, where g^μ is the metric-matrix element of a 5-dimensional space, given by $g^{\mu\nu} = (e_{11}, e_{22}, e_{33}, -e_{45}, -e_{54})$, where $e_{\mu\nu} = 1$ represents the non-zero matrix element. The invariants of g are $I_1 = P_\mu P^\mu$ and $I_2 = P_5$. Using the correspondence, $p_\mu = -i\hbar\partial_\mu$, and applying Ψ , we have:

$$\begin{cases} \partial_\mu \partial^\mu \Psi = k^2 \Psi \\ \partial_5 \Psi = -im\Psi \end{cases}, \quad (17)$$

where m is a constant and using $\Psi(x_\mu) = \exp(-imx_5)(\phi(\mathbf{x}, t))$, we obtain

$$-\frac{1}{2m}\nabla^2\phi(\mathbf{x}, t) = \left(i\partial_t + \frac{k^2}{2m}\right)\phi(\mathbf{x}, t), \quad (18)$$

which is the Schrödinger equation of a free particle of mass m and energy $E + \frac{k^2}{2m}$.

IV. THE PAULI-SCHRÖDINGER EQUATION

In this context, we present a construction of the spin wave equation 1/2, defining a new quadrivector γ^μ such that,

$$(\partial_\mu \partial^\mu - k^2) = (\gamma^\mu \partial_\mu + k)(\gamma^\nu \partial_\nu - k) \quad (19)$$

so, for Eq. (19) to be valid γ^μ must obey Clifford's algebra, that is,

$$\{\gamma^\mu, \gamma^\nu\} = 2g^{\mu\nu} \quad (20)$$

where $g^{\mu\nu}$ is our 5-dimensional metric.

Taking the positive part and acting on the wave function $\psi(x)$

$$(\gamma^\mu \partial_\mu + k)\psi(x) = 0 \quad (21)$$

For convenience, we will use the following representations of γ^μ

$$\gamma^i = \begin{pmatrix} \sigma^i & 0 \\ 0 & -\sigma^i \end{pmatrix}, \quad \gamma^4 = \begin{pmatrix} 0 & \sqrt{2} \\ 0 & 0 \end{pmatrix}, \quad (22)$$

$$\gamma^5 = \begin{pmatrix} 0 & 0 \\ -\sqrt{2} & 0 \end{pmatrix}; \quad (23)$$

where σ^i are the Pauli's matrices and $\sqrt{2}$ is the 2x2 identity matrix multiplied by $\sqrt{2}$.

Let $k = 0$ and adding a potential V , we have

$$\begin{pmatrix} \boldsymbol{\sigma} \cdot \mathbf{p} & -(E - V)\sqrt{2} \\ \sqrt{2}m & -\boldsymbol{\sigma} \cdot \mathbf{p} \end{pmatrix} \begin{pmatrix} \psi^L \\ \psi^S \end{pmatrix} = 0 \quad (24)$$

which leads us to

$$\boldsymbol{\sigma} \cdot \mathbf{p}\psi^L - (E - V)\sqrt{2}\psi^S = 0 \quad (25)$$

$$\boldsymbol{\sigma} \cdot \mathbf{p}\psi^S - \sqrt{2}m\psi^L = 0 \quad (26)$$

In Eq. (26) we have

$$\psi^L = \frac{\boldsymbol{\sigma} \cdot \mathbf{p}}{m\sqrt{2}}\psi^S \quad (27)$$

Substituting in Eq. (25) and using the fact $(\boldsymbol{\sigma} \cdot \mathbf{p})(\boldsymbol{\sigma} \cdot \mathbf{p}) = p^2$, we have

$$E\psi^L = \frac{p^2}{2m}\psi^L + V\psi^L \quad (28)$$

Similarly,

$$E\psi^S = \frac{p^2}{2m}\psi^S + V\psi^S \quad (29)$$

What is the Schrödinger equation for ψ^S and ψ^L respectively.

V. THE PAULI-HARTREE-FOCK EQUATION

The Hartree-Fock Equation is given by

$$f(1) = h(1) + \nu^{HF}(1) \quad (30)$$

where

$$h(1) = -\frac{1}{2}\nabla_1^2 - \sum_A \frac{Z_A}{r_{1A}} \quad (31)$$

and

$$\nu^{HF} = \sum_b J_b(1) - K_b(1) \quad (32)$$

Expanding ψ^L e ψ^S in their bases:

$$\psi^L = |\chi^L\rangle \mathbf{c}^L; \quad \psi^S = |\chi\rangle \mathbf{c}^S \quad (33)$$

Multiplying on the left by $(\langle\chi^L|, \langle\chi^S|)$, we have

$$\mathbf{\Pi}^{SS} \mathbf{c}^S = \sqrt{2}\mathbf{S}^{\mathbf{SL}} \mathbf{c}^L m \quad (34)$$

$$\mathbf{\Pi}^{LL} \mathbf{c}^L + \sqrt{2}\mathbf{V}^{\mathbf{LS}} \mathbf{c}^S = \sqrt{2}\mathbf{S}^{\mathbf{LS}} \mathbf{c}^S E^{LS} \quad (35)$$

where

$$\mathbf{\Pi}^{LL} = \langle \chi^L | \boldsymbol{\sigma} \cdot \mathbf{p} | \chi^L \rangle, \quad \mathbf{V}^{LS} = \langle \chi^L | V | \chi^S \rangle$$

$$\mathbf{S}^{LS} = \langle \chi^L | \chi^S \rangle.$$

Thus, our Fock matrix is

$$\mathbf{F} = \begin{bmatrix} \mathbf{F}^{LL} & \mathbf{F}^{LS} \\ \mathbf{F}^{SL} & \mathbf{F}^{SS} \end{bmatrix} \quad (36)$$

with

$$\begin{aligned} F_{\mu\nu}^{LL} &= \Pi_{\mu\nu}^{LL} + \sum_{\kappa\lambda} P_{\kappa\lambda}^{LL} [(\mu^L \nu^L | \kappa^L \lambda^L) - (\mu^L \lambda^L | \kappa^L \nu^L)] \\ &+ \sum_{\kappa\lambda} P_{\kappa\lambda}^{SS} [(\mu^L \nu^L | \kappa^S \lambda^S)] \\ F_{\mu\nu}^{LS} &= \sqrt{2} V_{\mu\nu}^{LS} - \sum_{\kappa\lambda} P_{\kappa\lambda}^{SL} (\mu^L \lambda^L | \kappa^S \nu^S) \\ F_{\mu\nu}^{SL} &= - \sum_{\kappa\lambda} P_{\kappa\lambda}^{LS} (\mu^S \lambda^S | \kappa^L \nu^L) \\ F_{\mu\nu}^{SS} &= \Pi_{\mu\nu}^{SS} + \sum_{\kappa\lambda} P_{\kappa\lambda}^{LL} (\mu^S \nu^S | \kappa^L \lambda^L) \\ &+ \sum_{\kappa\lambda} P_{\kappa\lambda}^{SS} [(\mu^S \nu^S | \kappa^S \lambda^S) - (\mu^S \lambda^S | \kappa^S \nu^S)] \end{aligned}$$

And of course the form of the PHF equations in Galilean covariance is the same in the case of the hartree-fock equation (with C as the e-arrays as eigenvalues)

$$\mathbf{FC} = \mathbf{SCE} \quad (37)$$

VI. THE MODIFIED PAULI EQUATION

Choosing the Ansatz,

$$\psi^S \equiv \frac{\boldsymbol{\sigma} \cdot \mathbf{p} \phi^L}{2\sqrt{2}mc^2}$$

where c is the velocity of light, replacing in the expression

$$\begin{pmatrix} \boldsymbol{\sigma} \cdot \mathbf{p} & -\sqrt{2}(E - V) \\ \sqrt{2}m & -\boldsymbol{\sigma} \cdot \mathbf{p} \end{pmatrix} \begin{pmatrix} \psi^L \\ \psi^S \end{pmatrix} = 0, \quad (38)$$

and rearranging terms, we have

$$\begin{pmatrix} \boldsymbol{\sigma} \cdot \mathbf{p} & \frac{V\boldsymbol{\sigma} \cdot \mathbf{p}}{2mc^2} \\ 0 & -\frac{p^2}{2\sqrt{2}mc^2} \end{pmatrix} \begin{pmatrix} \psi^L \\ \phi^L \end{pmatrix} = \begin{pmatrix} 0 & \frac{E\boldsymbol{\sigma} \cdot \mathbf{p}}{2mc^2} \\ -\sqrt{2}m & 0 \end{pmatrix} \begin{pmatrix} \psi^L \\ \phi^L \end{pmatrix} \quad (39)$$

Thus,

$$\boldsymbol{\sigma} \cdot \mathbf{p} \psi^L + \frac{V\boldsymbol{\sigma} \cdot \mathbf{p}}{2mc^2} \phi^L = \frac{E\boldsymbol{\sigma} \cdot \mathbf{p}}{2mc^2} \phi^L \quad (40)$$

$$p^2 \phi^L = 4m^2 c^2 \psi^L \quad (41)$$

Multiplying the first equation by $\frac{\boldsymbol{\sigma} \cdot \mathbf{p}}{2m}$ on the left, we have

$$\frac{p^2}{2m} \psi^L + \frac{(\boldsymbol{\sigma} \cdot \mathbf{p})V(\boldsymbol{\sigma} \cdot \mathbf{p})}{4m^2 c^2} \phi^L = E \psi^L \quad (42)$$

The only term remaining that has any spin dependence is the term involving the potential in Eq. (42), and this can also be separated out using the Pauli Matrices properties,

$$(\boldsymbol{\sigma} \cdot \mathbf{p})V(\boldsymbol{\sigma} \cdot \mathbf{p}) = \mathbf{p}V \cdot \mathbf{p} + i\boldsymbol{\sigma} \cdot \mathbf{p}V \times \mathbf{p}$$

It is now plain that the real spin dependence in the Dirac-like Pauli-Schrödinger equation is not in the kinetic energy, but in the potential for the small component—a fact that is hidden in our explicitly covariant form of the Pauli-Schrödinger equation. In an atomic system the potential is spherically symmetric, and we may write the spin-dependent term as

$$i\boldsymbol{\sigma} \cdot \mathbf{p}V \times \mathbf{p} = \frac{1}{r} \frac{\partial V}{\partial r} \hbar \boldsymbol{\sigma} \cdot \mathbf{r} \times \mathbf{p} = \frac{2}{r} \frac{\partial V}{\partial r} \mathbf{S} \cdot \mathbf{L} \quad (43)$$

By performing the spin separation, we have obtained a term that involves the interaction of the spin and the orbital angular momentum, a spin-orbit interaction.

VII. CONCLUSIONS

We began with a discussion of the Galilean Covariance. After, we showed the Galilean covariant Pauli-Schrödinger equation and we constructed the Galilean Dirac-Hartree-Fock-like equations; then propose a Hartree-Fock equation. Utilizing the modified Dirac-like equation, we also arrive at the spin-orbit coupling with the same g-factor found in relativistic mechanics.

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