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A derivation of the Pauli–Lenz vector and its variants

Kozo Kobayashi

Department of Physics, Saitama University, Urawa, Japan 338

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Abstract. Non-linear transformations of dynamic variables are used to extend a linear symmetry SO(3) of a quantum mechanical system to a larger one, SO(4). By making an application of this formalism to the hydrogen atom, the Pauli–Lenz vector and its variants are systematically derived.

1. Introduction

In view of the symmetry approach to quantum mechanics, the so-called Pauli–Lenz vector of the hydrogen atom is quite an interesting quantity. In quantum mechanics, the quantum numbers of a system are usually explained in terms of its manifest linear symmetries. For instance, the quantum numbers of the harmonic oscillators are given by their symmetries SU(n). The hydrogen atom has a symmetry SO(3) due to the spherically symmetric potential, by which its angular momenta are explained. However, its energy spectra are degenerate under the symmetry and cannot be explained by it. They are indeed connected with a dynamical symmetry SO(4) (Fock 1935, Bargmann 1936) which never manifests itself in the system.† The dynamical symmetry SO(4) is generated, together with the angular momentum, by the Pauli–Lenz vector

$$(-2H)^{-1/2}(\tfrac{1}{2}(\boldsymbol{J}\times\boldsymbol{p}-\boldsymbol{p}\times\boldsymbol{J})+\boldsymbol{x}/|\boldsymbol{x}|), \tag{1}$$

where H, $\boldsymbol{J}$, $\boldsymbol{p}$, $\boldsymbol{x}$ are the Hamiltonian, the angular momentum, the linear momentum and the relative coordinate respectively. (For simplicity, Planck's constant $\hbar$, the electron charge and the reduced mass will be set to unity throughout the paper.) This vector was derived by Pauli (1926), referring to the Runge–Lenz vector (Runge 1919, Lenz 1923) in the classical Kepler problem, and he first calculated the spectra of the hydrogen atom by using it. Since the vector was heuristically found by analogy with classical mechanics, the extended symmetry SO(4) was called a *hidden* symmetry and the degeneracy of the energy spectra under the manifest symmetry SO(3) an *accidental* one at that time (Fock 1935, Alliluev 1957).

To discover symmetries which are not obviously manifested in the Hamiltonian of a given system is physically and mathematically significant. This problem has been investigated by many authors. Niederer (1972, 1973) has studied the maximal kinematic invariance group of the free Schrödinger equation and of the harmonic oscillator. Boyer (1974) has carried out a similar analysis for an arbitrary potential. Miller (1977)

† For survey references to the Coulomb problem in quantum mechanics, see for example Biedenharn and Brussaard 1965, Mackintosh 1971, Englefield 1972.

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has developed a mathematically precise framework concerning symmetry and separation of variables. Goldstein (1975) has discussed the historical development of the discovery of the Runge–Lenz vector in classical mechanics, and Heintz (1974) has attempted its geometric determination. However, for the Pauli–Lenz vector in quantum mechanics, any systematic derivation has, to the author's knowledge, not been reported since Pauli's heuristic one (1926) which is based on analogy with the classical Runge–Lenz vector.

In the present paper, we will develop a formalism for enlarging a given linear symmetry through taking account of non-linear transformations of dynamic variables (§ 2) and will apply it to the hydrogen atom systematically to derive the Pauli–Lenz vector and its variants (§ 3). The non-linear transformation was first considered by Weinberg (1968) to discuss chiral dynamics in quantum field theory. The present work will suggest a useful application of the non-linear formalism to classical and quantum mechanics.

2. Non-linear extension of a linear symmetry SO(3) to SO(4)

Let us consider a three-dimensional quantum mechanical system which is described by the canonical coordinates x_a and momenta p_a $(a = 1, 2, 3)$ obeying the canonical quantisation rule

$$[x_a, p_b] = \mathrm{i}\delta_{ab}. \tag{2}$$

Suppose the system has a linear symmetry SO(3). That is, the system is invariant under the following linear transformations of the dynamic variables:

$$[J_a, x_b] = \mathrm{i}\epsilon_{abc}x_c, \tag{3a}$$

$$[J_a, p_b] = \mathrm{i}\epsilon_{abc}p_c, \tag{3b}$$

where J_a are the generators of SO(3) obeying the commutation relations

$$[J_a, J_b] = \mathrm{i}\epsilon_{abc}J_c, \tag{4}$$

and ϵ_{abc} is the totally antisymmetric tensor. (Throughout this paper, summation over repeated indices is understood.) The generators J_a are realised in terms of the dynamic variables as follows:

$$J_a = \epsilon_{abc}x_b p_c. \tag{5}$$

Now in order to extend the symmetry SO(3) to a larger one, SO(4), let us introduce three additional operators K_a which form, together with J_a, the Lie algebra of SO(4):

$$[J_a, K_b] = \mathrm{i}\epsilon_{abc}K_c, \tag{6}$$

$$[K_a, K_b] = \mathrm{i}\epsilon_{abc}J_c. \tag{7}$$

Then our question is whether such operators K_a can be realised out of the existing set of the dynamic variables. Once this is answered, the dynamical group SO(4) can be built in the system.

Let us study the realisation of K_a. Equation (6) tells us that the K_a form an SO(3) vector, which will be constructed out of the coordinates x_a, the momenta p_a and the

generators J_a. As is easily seen from the commutation relation (4), the J_a do not contribute to the K_a. Thus we can set

$$K_a = p_a f + x_a g, \tag{8}$$

where f, g are SO(3) scalars. The order of x_a, p_a and f, g in equation (8) is not unique; for instance, one might also take $K_a = f p_a + g x_a$. These formulations are essentially equivalent. Detailed properties of K_a are described by the commutation relations of f, g and x_a, p_a, which we write as follows:

$$[f, p_a] = \mathrm{i}(p_a F_1 + x_a F_2), \qquad [f, x_a] = -\mathrm{i}(x_a G_3 + p_a G_4), \tag{9a}$$

$$[g, p_a] = \mathrm{i}(p_a F_3 + x_a F_4), \qquad [g, x_a] = -\mathrm{i}(x_a G_1 + p_a G_2), \tag{9b}$$

where F_i, $G_i (i = 1, 2, 3, 4)$ are SO(3) scalars. These equations show that the operators K_a generate non-linear transformations of the dynamic variables. For the realisation (8), equation (7) yields the following constraint on f, g:

$$L \equiv \mathrm{i}[f, g] + (F_3 - F_2) f + (G_3 - G_2) g - 1 = 0. \tag{10}$$

Further, the quantisation rule (2) gives additional important relations: from the Jacobi identity of K_a, x_b, p_c, it follows that

$$F_3 = G_1, \qquad G_3 = F_1. \tag{11}$$

By taking into account these relations in equation (9), the functional form of f, g is specified as

$$(xp)(\xi(x^2) + \rho(p^2)) + \eta(x^2) + \sigma(p^2), \tag{12}$$

where the functions ξ, ρ, η, σ are subject to the constraint (10) and (xp), x^2, p^2 stand for $x_a p_a$, $x_a x_a$ and $p_a p_a$ respectively. The expression (12) for f, g is the result most characteristic of the present formulation.

3. Examples, and the Pauli–Lenz vector and its variants

In this section, we shall first present some examples of the general formulation developed in the preceding section. Next, applying them to the hydrogen atom, we shall carry out a non-linear extension of its symmetry SO(3) to SO(4) and derive the Pauli–Lenz vector and its variants.

3.1. Examples

3.1.1. Let f be

$$f = c(xp), \tag{13}$$

where c is a constant. According to equation (12), we write g as

$$g = (xp)(\xi + \rho) + \eta + \sigma.$$

From equation (10), it follows that

$$\xi = \rho = 0,$$

and η, σ are subject to the constraint

$$L = 2cx^2\eta' + c\eta - 2\eta\sigma' - 2cp^2\sigma' - 2\sigma\sigma' + c\sigma - 1 = 0, \tag{14}$$

where a prime denotes differentiation with respect to the argument x^2 or p^2. Thus we have

$$K_a = cp_a(xp) + x_a(\eta + \sigma). \tag{15}$$

3.1.2. Let us consider the case where the scalar functions f, g are given by the general polynomials of second order. (Ones of higher order would be given through non-linear transformations of the variables which leave the quantisation rule unchanged.) We write them as

$$f = f_1 + f_2x^2 + f_3(xp) + f_4p^2, \tag{16a}$$

$$g = g_1 + g_2p^2 + g_3(xp) + g_4x^2, \tag{16b}$$

where f_i, g_i $(i = 1, 2, 3, 4)$ are constants. The constraint (10) yields the following relations among them:

$L = 0$:

$$2f_1f_2 + 2g_1g_2 - f_1g_3 - g_1f_3 + 1 = 0, \tag{17a}$$

$$2f_2^2 + f_2g_3 + 2g_2g_4 - 3f_3g_4 = 0, \tag{17b}$$

$$2g_2^2 + g_2f_3 + 2f_2f_4 - 3g_3f_4 = 0, \tag{17c}$$

$$f_2f_3 + g_2g_3 - f_3g_3 = 0, \tag{17d}$$

$$f_2g_2 - f_4g_4 = 0. \tag{17e}$$

With these f_i, g_i,

$$K_a = p_a(f_1 + f_2x^2 + f_3(xp) + f_4p^2) + x_a(g_1 + g_2p^2 + g_3(xp) + g_4x^2). \tag{18}$$

3.1.3. Let f be a function of x^2:

$$f = f(x^2). \tag{19}$$

From equation (10), we have

$$\rho = \sigma = 0,$$

and

$$\xi = \frac{2ff' + 1}{f - 2x^2f'} \qquad (f \neq 0, \text{const} \times \sqrt{x^2}). \tag{20}$$

The result is

$$g = (xp)\xi + \eta, \qquad (\eta \text{ arbitrary})$$

$$K_a = p_af + x_a((xp)\xi + \eta). \tag{21}$$

3.2. The Pauli–Lenz vector and its variants

Let us apply the above results to the hydrogen atom. All the examples given above will turn out to yield the Pauli–Lenz vector or its variants if the invariance with respect to the Hamiltonian is imposed. The Hamiltonian H is given by

$$H = \tfrac{1}{2}p^2 - 1/\sqrt{x^2}. \tag{22}$$

Since we concern ourselves with the bound states, H is assumed to be a negative constant in the following.

In example 3.1.1, the invariance of the operator (15) specifies η, σ as

$$\eta = c(x^2)^{-1/2}, \qquad \sigma = -cp^2.$$

Then equation (14), which manifests a structure of the group SO(4) in the present example, becomes

$$\tfrac{1}{2}p^2 - 1/\sqrt{x^2} + 1/2c^2 = 0.$$

This is nothing other than the Hamiltonian (22) with $c = (-1/2H)^{1/2}$. Thus K_a is given as

$$K_a = (-2H)^{-1/2}(p_a(xp) + \frac{x_a}{\sqrt{x^2}}(1-p^2)),$$

$$= (-2H)^{-1/2}(\tfrac{1}{2}(\boldsymbol{J}\times\boldsymbol{p} - \boldsymbol{p}\times\boldsymbol{J}) + \boldsymbol{x}/\sqrt{\boldsymbol{x}^2})_a.$$

This is just the Pauli–Lenz vector (1).

For example 3.1.2, in order to obtain an invariant K_a, we must slightly modify the Hamiltonian; the use of equation (22) gives a trivial solution $K_a = 0$. The quantisation rule (2) allows the scale transformation of the dynamic variables:

$$x_a \to s\tilde{x}_a, \qquad p_a \to s^{-1}\tilde{p}_a,$$

where s is a scale parameter. By taking $s = (-2H)^{1/2}$, the Hamiltonian (22) is written as

$$\sqrt{\tilde{x}^2}(1+\tilde{p}^2) = 2/s = (2/(-H))^{1/2}. \tag{23}$$

Since for the states diagonalising H the LHS replaces the Hamiltonian, let us determine the invariant $\tilde{K}_a$ by equation (23):

$$[\sqrt{\tilde{x}^2}(1+\tilde{p}^2), \tilde{K}_a] = 0.$$

We have then

$$f_3 = 2g_1, \qquad g_2 = -g_1,$$

other coefficients vanishing. Further, from equation (17), it follows that

$$g_1 = \tfrac{1}{2}, \qquad g_2 = -\tfrac{1}{2}, \qquad f_3 = 1.$$

Thus

$$\tilde{K}_a = \tfrac{1}{2}\tilde{x}_a(1-\tilde{p}^2) + \tilde{p}_a(\tilde{x}\tilde{p}),$$

$$= \tfrac{1}{2}(\tilde{\boldsymbol{J}}\times\tilde{\boldsymbol{p}} - \tilde{\boldsymbol{p}}\times\tilde{\boldsymbol{J}} + \tilde{\boldsymbol{x}}(1+\tilde{p}^2))_a. \tag{24}$$

Taking account of $1+\tilde{p}^2 = 2/s\sqrt{\tilde{x}^2}$, (equation (23)), and rewriting it in the original variables, we easily verify that equation (24) reproduces the Pauli–Lenz vector. Thus it gives a polynomial-type variant of the Pauli–Lenz vector.

For equation (21) of example 3.1.3, we make a unitary transformation

$$\tilde{x}_a \to \tilde{p}_a, \qquad \tilde{p}_a \to -\tilde{x}_a,$$

which leaves the quantisation rule unchanged. Then the invariance with respect to the Hamiltonian (23) yields just the same $\tilde{K}_a$ as the above equation (24). Thus this one is also another polynomial-type variant of the Pauli–Lenz vector.

For any explicitly given f, we could in a similar manner obtain the corresponding additional operators K_a for extending the given linear symmetry. As is seen through the above examples, these operators seem to reproduce the Pauli–Lenz vector or its variants under the invariance condition with respect to the Hamiltonian of the system.

4. Concluding remarks

In quantum theory, quantum numbers of a system are usually explained in terms of its linear invariant groups. As is seen in recent high-energy physics, with development of experimental and theoretical studies, more and more new quantum numbers are found, and it becomes impossible for the groups to accommodate them. The most conventional way in which physicists have dealt with these new quantum numbers has been the introduction of new additional degrees of freedom (fields or particles) so as *linearly* to extend the symmetries. This procedure is however not complete: the number of unknowns is never lessened because of the introduction of the hypothetical degrees of freedom. Although there have been a number of successes of this sort in the history of high-energy physics, recent compound models of elementary particles suffer from this serious problem, and the confinement of the assumed basic fields is extensively discussed nowadays (see e.g. Marciano and Pagels 1978). In this connection, it should be noticed that the introduction of new degrees of freedom in the system is not always necessary in order to enlarge its invariance groups, if one takes into consideration non-linear transformations of the dynamic variables. Such a situation can typically be observed in the dynamics of the hydrogen atom. In the present work, for the Coulomb problem in quantum mechanics which has a manifest symmetry SO(3), the extra generators of a larger dynamical symmetry SO(4) have been realised non-linearly on the existing set of dynamic variables. This is nothing other than the so-called Pauli–Lenz vector for the hydrogen atom.

Our formalism could in a straightforward way be generalised to the non-linear extension of a linear symmetry SO(n) to SO($n+1$) for quantum mechanial systems, and also for classical ones if one translates it into the classical version.

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