GAUGE–INDEPENDENT THEORY OF SYMMETRY. II

By H. A. Buchdahl* and L. J. Tassie*

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Summary

This paper develops a gauge-independent symmetry theory of non-relativistic quantum mechanical systems, in line with that previously considered in the context of classical mechanics. We first discuss at length the motivation for adopting the view that the invariance of a system K under a physical symmetry operation $\mathscr{S}$ should be taken to mean invariance of the equation of motion of K under a certain gauge-independent unitary transformation $U_c(\mathscr{S})$. The formal development of the theory is then carried through, and some detailed examples are presented. In particular, corresponding to every direction along which a system K happens to be translation invariant there exists a gauge-independent generator of translations which leaves K invariant but which is not, in general, a component of either the canonical or the kinetic momentum. The connexion between such invariant generators of translations and the so-called magnetic translation operators is referred to.

I. Introduction

In a previous paper (Tassie and Buchdahl 1964) hereafter referred to as I, we considered, in the context of classical dynamics, the problem of defining in a gauge-independent way the condition that a system be invariant under some symmetry operation. We now go on to consider this question in the context of non-relativistic quantum mechanics.

If U is a time-independent (unitary) operator which leaves the Hamiltonian $H(p,q,t)$ of a dynamical system K invariant,

$$UHU^{-1} = H, \tag{1.1}$$

then U is a constant of the motion. Therefore, writing

$$U = \mathrm{e}^{\mathrm{i}G}, \tag{1.2}$$

if U is an element of a continuous group, the observable G is conserved. One says that K has the symmetry $\mathscr{S}$, or admits the symmetry operation $\mathscr{S}$, of which U is the image in Hilbert space. It is therefore usually stated that the condition

$$[U,H] = 0 \tag{1.3}$$

is a condition for the symmetry of K under $\mathscr{S}$. Now it is certainly true that the condition is *sufficient*. However, it is sometimes made to appear, at least by implication, that the condition is also *necessary*. Whether this is true or not depends on certain questions of definition, in the sense that one must first say what is meant by (i) the invariance of K under an operation $\mathscr{O}$; (ii) "momentum".

* Department of Theoretical Physics, School of General Studies, Australian National University, Canberra.

$\mathcal{O}$ is to be regarded as a physical operation in which K is shifted rigidly in such a way that the initial coordinates x_k ($k = 1, 2, 3$) of any element of K become*

$$x'_k = a_{kl}\, x_l + a_k \tag{1.4}$$

as a consequence of $\mathcal{O}$. (Summation over repeated indices is implied.) Here a_{kl}, a_k are constants, the a_{kl} being the coefficients of an orthogonal transformation, so that

$$a_{km}\, a_{lm} = a_{mk}\, a_{ml} = \delta_{kl}. \tag{1.5}$$

One may then *lay down* that the image U of $\mathcal{O}$ shall be such that if the x_k are now coordinate operators then

$$U x_k\, U^{-1} = x'_k, \tag{1.6}$$

(1.4) being retained. Observe now that the effect of U on the "canonical momenta" p_k is not uniquely defined. All one knows is that the x_k, p_l obey the canonical commutation relations†

$$[x_k, x_l] = 0, \qquad [p_k, p_l] = 0, \qquad [x_k, p_l] = \mathrm{i}\delta_{kl}, \tag{1.7}$$

and likewise

$$[x'_k, x'_l] = 0, \qquad [p'_k, p'_l] = 0, \qquad [x'_k, p'_l] = \mathrm{i}\delta_{kl}. \tag{1.8}$$

The necessary and sufficient condition for the compatibility of equations (1.4)–(1.8) is that

$$p'_k = U p_k\, U^{-1} = a_{kl}\{p_l + \partial f(x,t)/\partial x_l\}, \tag{1.9}$$

where the function f of the coordinates and of the time remains arbitrary.‡ To this extent the canonical momentum p_k is not uniquely defined; its precise nature depends in any particular case upon the "gauge function" f.

That we do not now choose $f = 0$ once and for all is no mere act of pedantry. Consider the case when K is a particle of mass m and charge** ce in an electromagnetic field whose potentials are $\mathbf{A}$, Φ, so that

$$H = \frac{1}{2m}(\mathbf{p} - e\mathbf{A}) \cdot (\mathbf{p} - e\mathbf{A}) + ce\Phi. \tag{1.10}$$

Then

$$m\dot{x}_k = m[x_k, H] = p_k - eA_k. \tag{1.11}$$

Suppose now in particular that the field strengths are zero and that $\mathcal{O}$ is an infinitesimal translation through $\boldsymbol{\varepsilon}$:

$$a_{kl} = \delta_{kl}, \qquad a_k = \epsilon_k. \tag{1.12}$$

Then

$$\begin{aligned} m\dot{x}'_k &= p'_k - eA_k(x_s + \epsilon_s, t) \\ &= p'_k - e\{A_k(x_s, t) + \epsilon_r\, \partial A_k(x_s, t)/\partial x_r\}. \end{aligned}$$

* In the case of the parity operation this statement has to be interpreted appropriately.

† $\hbar$ has been taken as unity.

‡ Spin is here being disregarded.

** That is, e is the electronic charge divided by the speed of light c.

One must surely require for a free particle that

$$\dot{x}_k' = \dot{x}_k, \tag{1.13}$$

so that

$$p_k' - p_k = e\epsilon_r \,\partial A_k/\partial x_r = \partial(e\epsilon_r A_r)/\partial x_k,$$

since $\partial A_k/\partial x_r = \partial A_r/\partial x_k$, and therefore here

$$f = e\boldsymbol{\varepsilon} \,.\, \mathbf{A}. \tag{1.14}$$

Of course, this conclusion is bound up with the fact that the potentials need not be zero even when the electromagnetic field $\mathscr{E}$, $\mathscr{H}$ is zero, that is to say, with the gauge invariance of Maxwell's equations.

We continue in terms of the present example. It is commonly stated (e.g. Messiah 1962, p. 652) that "$\boldsymbol{\varepsilon} \,.\, \mathbf{p}$ is the generator of translations", i.e. of the infinitesimal displacement $\boldsymbol{\varepsilon}$ ($U = 1 + i\boldsymbol{\varepsilon} \,.\, \mathbf{p}$). Presumably one has to understand here that $H(\mathbf{p}, \mathbf{x}, t)$ is given and the operators $\mathbf{p}$ in U are the same as these which occur in H. The mistake here lies in referring to $\boldsymbol{\varepsilon} \,.\, \mathbf{p}$ as *the* rather than as *a* generator of translation. For clearly $U\mathbf{p}U^{-1} = \mathbf{p}$, which is at variance with (1.9) and (1.14). Indeed, granted (1.10) *and* (1.13) one has to take $\boldsymbol{\varepsilon} \,.\, (\mathbf{p} - e\mathbf{A})$ as the appropriate generator of translations.

In short, granted that a free particle (i.e. one on which no forces are acting) is to be regarded as a system invariant under translations, the generator of translations is $\boldsymbol{\varepsilon} \,.\, (\mathbf{p} - e\mathbf{A})$. Note that (i) $\mathbf{p} - e\mathbf{A}$ is the kinetic momentum $m\dot{\mathbf{x}}$; (ii) $\mathbf{p} - e\mathbf{A}$, but not $\mathbf{p}$, is conserved; (iii) in general neither $\mathbf{p}$ nor $\mathbf{p} - e\mathbf{A}$ commute with H and, in general, they are not conserved. We are now ready to consider the general problem, and this will be done in the following sections.

II. Symmetry Operations

By considering the special case of translations we saw that it is not desirable to take invariance of a system K under a symmetry operation $\mathscr{S}$ to mean simply the invariance of the Hamiltonian H under some unitary transformation U which is the image of $\mathscr{S}$ in Hilbert space. On the contrary all that is necessary on physical grounds is that *the equations of motion of K shall be invariant under $\mathscr{S}$*. This, then, is the answer to one of the questions asked above. Only rarely is the sufficiency of this condition recognized explicitly; but even when it is (Messiah 1962, p. 661) its relevance to gauge independence does not appear to have been adequately pursued. It is true that by a suitable choice of gauge one can arrange H to be invariant under the unitary image of any selected *one-parameter* continuous subgroup of a given r-parameter ($r > 1$) continuous group $\mathscr{O}$ of operations. One cannot, however, always achieve the invariance of H for more than one subgroup at a time. On the contrary, one has to re-gauge on proceeding from one subgroup to the next. This is incidentally the situation one has when the manifest covariance of electrodynamics is destroyed by adoption of the Coulomb gauge. The theory is still (manifestly) covariant with respect to spatial rotations, but one has to go over to a new gauge after the performance of every Lorentz transformation. Again, a particle travelling in a homogeneous magnetic field $\mathscr{H}$ must surely be regarded as a system invariant under rotations about *any* axis parallel to $\mathscr{H}$. Yet if $\mathbf{A}$ is symmetric about one such axis it will not be symmetric about any other. In every case the conclusion is the same, namely, that one should have a gauge-invariant definition of symmetry. We turn now to the formal aspects of the problem.

III. Invariance of the Equation of Motion

In the Schrödinger picture the equation of motion of K is

$$H|\rangle = \mathrm{i}\,\mathrm{d}|\rangle/\mathrm{d}t. \tag{3.1}$$

Under an arbitrary canonical transformation U this becomes

$$H^*|^*\rangle = \mathrm{i}\,\mathrm{d}|^*\rangle/\mathrm{d}t, \tag{3.2}$$

where $|^*\rangle = U|\rangle$, and the transformed time displacement operator H^* is given by

$$H^* = UHU^\dagger + \mathrm{i}\frac{\partial U}{\partial t}U^\dagger . \tag{3.3}$$

Now if U is any particular chosen image of the operation $\mathscr{O}$ to which (1.4) and (1.6) relate, then we know from Section I that any other image of $\mathscr{O}$ must have the form CU, where

$$C = \mathrm{e}^{\mathrm{i}f(x,t)} \tag{3.4}$$

is a unitary operator which is a function of x and t only.

If $\mathscr{O}$ is in fact a symmetry operation $\mathscr{S}$, it must be possible to choose C such that H^* is identical with H. With *this* choice of C we write

$$U_c = CU. \tag{3.5}$$

Accordingly, formally replacing U by U_c and H^* by H in (3.3) it follows that we must have

$$\frac{\partial U_c}{\partial t} + \mathrm{i}[H, U_c] = 0. \tag{3.6}$$

Evidently U_c is conserved. Using (3.4), equation (3.6) may be written in the form

$$\frac{\partial f}{\partial t} + \mathrm{e}^{-\mathrm{i}f}H\mathrm{e}^{\mathrm{i}f} = \mathrm{i}\frac{\partial U}{\partial t}U^\dagger + UHU^\dagger. \tag{3.7}$$

Thus, if a function $f(x,t)$ can be found which satisfies (3.7) then the equation of motion of K is invariant under the transformation (1.4). Amongst all possible operators which have the common property that they induce (1.4), U_c occupies a special position for (i) it is the true symmetry operator corresponding to $\mathscr{S}$ in the sense that it leaves the equation of motion of K invariant; (ii) it is conserved. U_c may be called the *invariant image of* $\mathscr{S}$; and if $\mathscr{S}$ is an element of a continuous group one has the corresponding *invariant generator of* $\mathscr{S}$.

IV. Translations, Rotations, Inversions

(a) *Translations*

Take

$$G = \boldsymbol{\varepsilon} \,.\, \mathbf{p} \tag{4.1}$$

as a generator of an infinitesimal translation $\boldsymbol{\varepsilon}$. The lack of uniqueness of G is now irrelevant since our results must be independent of any particular choice from amongst all possible generators. Although there is great formal similarity between the classical and the quantum mechanical results we shall reconsider the examples of I in some detail.

Write

$$f = \epsilon g, \tag{4.2}$$

where ϵ is the magnitude of $\boldsymbol{\varepsilon}$. Then from (3.7), if K is to be invariant under the translation $\boldsymbol{\varepsilon}$, ϵg must satisfy the equation

$$[\boldsymbol{\varepsilon}_0 \,.\, \mathbf{p}+g, H]+\mathrm{i}\, \partial g/\partial t = 0, \qquad (\boldsymbol{\varepsilon}_0 = \boldsymbol{\varepsilon}/\epsilon). \tag{4.3}$$

Using (1.10) this becomes explicitly

$$\frac{1}{2m}\left[(\mathbf{p}-e\mathbf{A}),\, \left(e\frac{\mathrm{d}\mathbf{A}}{\mathrm{d}s} + \operatorname{grad} g\right)\right]_+ - ce\frac{\mathrm{d}\Phi}{\mathrm{d}s} + \frac{\partial g}{\partial t} = 0,$$

where $\mathrm{d}/\mathrm{d}s$ denotes spatial differentiation along the direction of $\boldsymbol{\varepsilon}$, whilst for any two vectors $\mathbf{C}$ and $\mathbf{D}$

$$[\mathbf{C}, \mathbf{D}]_+ \equiv \mathbf{C} \,.\, \mathbf{D}+\mathbf{D} \,.\, \mathbf{C}. \tag{4.4}$$

The factor multiplying $\mathbf{p}$ must vanish, and so

$$\operatorname{grad} g = -e\,\mathrm{d}\mathbf{A}/\mathrm{d}s, \qquad \partial g/\partial t = ce\,\mathrm{d}\Phi/\mathrm{d}s. \tag{4.5}$$

These are integrable if, and only if,

$$\mathrm{d}\mathscr{E}/\mathrm{d}s = \mathrm{d}\mathscr{H}/\mathrm{d}s = 0, \tag{4.6}$$

that is, $\mathscr{E}$ and $\mathscr{H}$ must not vary along the direction of the translation. When these conditions are satisfied (4.5) give the total differential of g, and one may proceed as in I. Thus

$$\mathrm{d}g = e\boldsymbol{\varepsilon}_0 \,.\, (-\,\mathrm{d}\mathbf{A}+\mathscr{H}\times \mathrm{d}\mathbf{x}-c\mathscr{E}\,\mathrm{d}t), \tag{4.7}$$

which may be integrated along any convenient contour. The result is of the form

$$g = \boldsymbol{\varepsilon}_0 \,.\, (-e\mathbf{A}+\mathfrak{g}), \tag{4.8}$$

with

$$\mathfrak{g} = e \int (\mathscr{H}\times \mathrm{d}\mathbf{x}-c\mathscr{E}\mathrm{d}t). \tag{4.9}$$

The invariant generator of translations is therefore

$$\begin{aligned}\Gamma = \boldsymbol{\varepsilon} \,.\, \mathbf{p}+\epsilon g &= \boldsymbol{\varepsilon} \,.\, \{(\mathbf{p}-e\mathbf{A})+\mathfrak{g}\}\\ &= \boldsymbol{\varepsilon} \,.\, (m\dot{\mathbf{x}}+\mathfrak{g}).\end{aligned} \tag{4.10}$$

The gauge invariance of Γ is evident on inspection. Note that, in general, this is neither the canonical nor the kinetic component of momentum in the direction $\boldsymbol{\varepsilon}_0$.

Accordingly it will, as in I, be called a component of *symmetry momentum*. It should be carefully observed that, the terminology notwithstanding, it is defined only when (4.6) is satisfied.

If K is invariant under translations along two different directions, one essentially doubles the number of equations above. Formally one need only supply the symbols $\boldsymbol{\varepsilon}$, g, and s with alternative subscripts 1 and 2. In particular $\mathscr{E}$ and $\mathscr{H}$ must not vary along the direction of $\boldsymbol{\varepsilon}_1$ or $\boldsymbol{\varepsilon}_2$. It should be noted that an electromagnetic gauge transformation can be arranged so as to make *one* of the invariant generators a component of canonical momentum. In general one cannot, however, make both invariant generators canonical. The detailed discussion of this case, or the case of invariance along three distinct directions, is much the same as that given in I.

(*b*) *Rotations*

It suffices to consider rotations about the z-axis. The generator of an infinitesimal rotation through the angle ϵ is

$$G = \epsilon L_z = \epsilon(xp_y - yp_x). \tag{4.11}$$

As in the case of (4.1) the lack of uniqueness of this is irrelevant. We take the case referred to at the end of Section II, i.e. that of the homogeneous magnetic field $\mathscr{H} = (0, 0, \mathscr{H})$, $\mathscr{E} = 0$. In particular, one can certainly choose the gauge so as to make the Hamiltonian invariant under rotations about any particular axis along the direction of $\mathscr{H}$; but then it will not be invariant under rotations about any other axis parallel to the first.

The equation corresponding to (4.3) is

$$[L_z + g, H] + \mathrm{i}\,\partial g/\partial t = 0. \tag{4.12}$$

Explicitly this reads

$$-\frac{e}{2m}\{[p_y, A_x]_+ - [p_x, A_y]_+ + [\mathbf{p}, D\mathbf{A}]_+\}$$
$$+\frac{1}{2m}[(\mathbf{p} - e\mathbf{A}),\ \operatorname{grad} g]_+ + ceD\Phi + \frac{e^2}{2m}D|\mathbf{A}|^2 + \frac{\partial g}{\partial t} = 0,$$

where D stands for $y\,\partial/\partial x - x\,\partial/\partial y$. The factor multiplying $\mathbf{p}$ must vanish, and so

$$\partial g/\partial x = e(DA_x - A_y), \qquad \partial g/\partial y = e(DA_y + A_x),$$
$$\partial g/\partial z = eDA_z, \qquad \partial g/\partial t = -ceD\Phi, \tag{4.13}$$

where the last equation has been simplified by means of the expression for $\operatorname{grad} g$ provided by the first three. The integrability conditions on (4.13) are satisfied, and one finds easily that

$$g = e(yA_x - xA_y) + \tfrac{1}{2}\mathscr{H}(x^2 + y^2). \tag{4.14}$$

The invariant generator of two-dimensional rotations is therefore

$$\Gamma = \epsilon(L_z + g) = \epsilon\{x(p_y - eA_y) - y(p_x - eA_x) + \mathfrak{g}\}, \tag{4.15}$$

with

$$\mathfrak{g} = \tfrac{1}{2}e\mathscr{H}(x^2 + y^2). \tag{4.16}$$

The conserved observable is thus Γ/ϵ, that is, the (component of) *symmetry angular momentum*

$$P_z = m(\mathbf{r}\times\dot{\mathbf{r}})_z+\tfrac{1}{2}e\mathscr{H}(x^2+y^2). \tag{4.17}$$

Once again it should be carefully noted that P_z is neither a canonical nor a kinetic component of angular momentum; and that it does not necessarily commute with the Hamiltonian.

(c) *Inversions*

Inversions, that is to say the parity operation, correspond to the choice

$$a_{kl} = -\delta_{kl}, \qquad a_k = 0 \tag{4.18}$$

in (1.4). Thus

$$U\mathbf{r}U^{-1} = -\mathbf{r}. \tag{4.19}$$

From (4.19) it does not follow that

$$U\mathbf{p}U^{-1} = -\mathbf{p}, \tag{4.20}$$

as we know from Section I. (In the literature it is generally made to appear (e.g. Merzbacher 1961; Kurşunoğlu 1962) as if one were *forced* to lay down (4.20) as well as (4.19).) However, in our gauge-independent formalism (4.20) may be adopted without anything thus being lost, provided one adheres to that definition of the symmetry of K under U which follows equation (3.7).

If $F(\mathbf{r},t)$ is any function of $\mathbf{r}$, t, we shall take F_- to mean $F(-\mathbf{r},t)$; whilst occasionally $F(\mathbf{r},t)$ itself will be written as F_+ for emphasis. Recalling (3.4), equation (3.7) now reads

$$\tfrac{1}{2}m\{|\mathbf{p}+e\mathbf{A}_- - \operatorname{grad} f|^2 - |\mathbf{p}-e\mathbf{A}_+|^2\}+ce(\Phi_- - \Phi_+) - \partial f/\partial t = 0,$$

which, in the usual way, requires

$$\begin{aligned}\operatorname{grad} f &= e(\mathbf{A}_+ + \mathbf{A}_-),\\ \partial f/\partial t &= -ce(\Phi_+ - \Phi_-).\end{aligned} \tag{4.21}$$

The integrability conditions on (4.21) are

$$\mathscr{H}_- = \mathscr{H}_+, \qquad \mathscr{E}_- = -\mathscr{E}_+. \tag{4.22}$$

When these are satisfied f may be determined from (4.21). The true parity operator ("true" in the sense indicated at the end of Section III) is then

$$U_c = \mathrm{e}^{\mathrm{i}f}U, \tag{4.23}$$

and this is conserved.

V. Concluding Remarks

The program outlined in Section I has been illustrated by the preceding examples, and it remains only to recapitulate the main point. It is this: the idea that invariance of a system K under a physical symmetry operation $\mathscr{S}$ means invariance of the Hamiltonian H of K under some particular image $U(\mathscr{S})$ of $\mathscr{S}$ in Hilbert space is in general too narrow, since this "invariance" could be destroyed by a physically empty gauge transformation. We have therefore taken invariance to mean invariance of the equation of motion of K, in which case one is led to a *gauge-invariant* image of $\mathscr{S}$, whenever K is in fact invariant under $\mathscr{S}$ in the sense now adopted.

It may be apposite to enlarge these remarks somewhat with regards to the special case of translations. If K is invariant under translations in the direction $\boldsymbol{\varepsilon}_0$, then there exists a corresponding component of symmetry momentum Γ (see equation (4.10)), which is the invariant generator for this symmetry operation. If one has translation invariance along two distinct directions $\boldsymbol{\varepsilon}_{01}$ and $\boldsymbol{\varepsilon}_{02}$, then there exist the two corresponding invariant generators Γ_1, Γ_2. Further, Γ_1 and Γ_2 will, in general, fail to commute. It follows incidentally that these generators do not form a representation of the translation group,* but only a ray-representation, i.e. a representation to within a phase factor. If one has invariance along three linearly independent directions, one has a set of three invariant generators and these then form a ray-representation of the full translation group.

In this special situation the invariant generators have been previously defined by Brown (1964) who, however, uses a special gauge. In the presence of a homogeneous magnetic field he chooses a gauge such that

$$\mathbf{A} = \tfrac{1}{2}\mathscr{H}\times\mathbf{r}. \tag{5.1}$$

He then defines what he calls "magnetic translation operators" which, transcribed into the present terminology, correspond to taking

$$\boldsymbol{\Gamma} = \boldsymbol{\varepsilon}\,.\,(\mathbf{p}+e\mathbf{A}). \tag{5.2}$$

Without any particular choice of gauge, on the other hand, we have from (4.9)

$$\boldsymbol{\Gamma} = \boldsymbol{\varepsilon}\,.\,(\mathbf{p}-e\mathbf{A}+e\mathscr{H}\times\mathbf{r}), \tag{5.3}$$

and this naturally reduces to (5.2) when (5.1) is adopted.

A final remark concerns the behaviour of expectation values under a symmetry operation $\mathscr{S}$. The point at issue is sufficiently illustrated by considering the specific case of a rotation $\mathscr{R}$. One normally understands V_1, V_2, V_3 $(=\mathbf{V})$ to be the components of a vector operator if under $\mathscr{R}$ they transform according to

$$\tilde{U}V_j\tilde{U}^\dagger = R_{jk}V_k, \tag{5.4}$$

where $\tilde{U}$ is a unitary image of $\mathscr{R}$. Then the expectation value of $\mathbf{V}$ transforms as a vector under spatial rotations. Making the definite choice $\tilde{U} = U_c$ we see that $\mathbf{r}$, for instance, is a vector operator. However, in general

$$U_c p_j U_c^\dagger \neq R_{jk}p_k,$$

(see equation (1.9)) so that $\mathbf{p}$ is not a vector operator according to the usual definition. A particle velocity $\mathbf{v}$ on the other hand is a vector operator, for $\mathbf{v} = im^{-1}[H,\mathbf{r}]$ in which $\mathbf{r}$ is a vector operator, whilst H goes into itself under transformation by U_c.

* Here, the group of plane translations in the direction of $a\boldsymbol{\varepsilon}_{01}+b\boldsymbol{\varepsilon}_{02}$, with arbitrary a and b.

All this amounts to saying that covariance under $\mathscr{S}$ is to be required only for gauge-invariant dynamical variables, whilst canonical momenta or other gauge-variant variables are covariant only to within gauge transformations.

VI. References

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