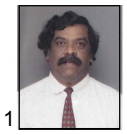
Symmetries and Conservation Laws in Classical and Quantum Mechanics

2. Quantum Mechanics

K S Mallesh, S Chaturvedi, V Balakrishnan, R Simon and N Mukunda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K S Mallesh – his interests are density matrix techniques, polarization and spin squeezing.

Subhash Chaturvedi – his current research interests include phase space descriptions of finite state quantum systems and quantum information theory.

V Balakrishnan – his research interests are statistical physics, stochastic processes and dynamical systems.

R Simon – his research interests are in quantum information science and quantum optics.

N Mukunda – his interests are classical and quantum mechanics, theoretical optics and mathematical physics.

In Part 1 of this two-part article we have spelt out, in some detail, the link between symmetries and conservation principles in the Lagrangian and Hamiltonian formulations of classical mechanics (CM). In this second part, we turn our attention to the corresponding question in quantum mechanics (QM). The generalization we embark upon will proceed in two directions: from the classical formulation to the quantum mechanical one, and from a single (infinitesimal) symmetry to a multi-dimensional Lie group of symmetries. Of course, we always have some definite physical system in mind. We also assume that the reader is familiar with the elements of quantum mechanics at the level of a standard first course on the subject. Operators will be denoted with an overhead caret, e.g., $\hat{A}$, $\hat{G}$, $\hat{U}$, etc., while $[\hat{A}\,,\,\hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$ is the commutator of $\hat{A}$ and $\hat{B}$.

1. Symmetry in Quantum Mechanics

The treatment of symmetry and invariance in QM is closely modelled on the Hamiltonian formalism in CM. As is well known, we have the formal replacements

- Poisson bracket (PB) in CM $\rightarrow$ commutator$/(i\hbar)$ in QM.
- Canonical transformation (CT) in phase space $\rightarrow$ unitary transformation (UT) on Hilbert space.

These statements will be qualified and elaborated upon,

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subsequently. Corresponding to any continuous symmetry of a quantum system, we have a constant of the motion (COM) that is now a hermitian operator $\hat{G}$. A finite symmetry transformation, as opposed to an infinitesimal one, is represented by a UT built up from a succession of infinitesimal transformations. It has the general form

$$\hat{U}(\alpha) = \mathrm{e}^{-i\alpha\,\hat{G}/\hbar}. \tag{1}$$

Here, $\hat{G}$ is the *infinitesimal generator* (often abbreviated to simply 'the generator') of the transformation, and α is the (real) parameter characterising the transformation. The constant $\hbar$ has been introduced explicitly in the exponent in (1) for convenience – this is the form in which unitary transformations commonly occur in QM. Note that the product $(\alpha\,\hat{G})$ has the same physical dimensions as $\hbar$, i.e., those of angular momentum, or (length) $\times$ (linear momentum). The effects of the transformation on state vectors (or wave functions) and on dynamical variables, respectively, are given by

$$|\Psi\rangle \rightarrow |\Psi\,'\rangle = \hat{U}(\alpha)|\Psi\rangle, \tag{2a}$$

$$\hat{A} \rightarrow \hat{A}' = \hat{U}(\alpha)\,\hat{A}\,\hat{U}^{-1}(\alpha). \tag{2b}$$

Since $\hat{G}$ is hermitian and $\hat{U}(\alpha)$ is unitary, we have

$$\hat{U}^{-1}(\alpha) = \hat{U}^{\dagger}(\alpha) = \mathrm{e}^{i\alpha\,\hat{G}/\hbar}. \tag{3}$$

A combination like $\hat{U}\,\hat{A}\,\hat{U}^{-1}$ is called the *conjugation* of $\hat{A}$ by $\hat{U}$.

The equation of motion (EOM) in quantum mechanics is the Schrödinger equation for the state vector of a system, namely,

$$i\hbar\,\frac{\mathrm{d}|\Psi(t)\rangle}{\mathrm{d}t} = \hat{H}(t)|\Psi(t)\rangle, \tag{4}$$

where $\hat{H}(t)$ is the Hamiltonian of the system. For generality, we have allowed for a possible explicit time-dependence in $\hat{H}$. Now, a dynamical variable $\hat{G}(t)$ with

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Even when a constant of the motion has an explicit time dependence, the corresponding unitary transformation preserves the Schrödinger equation.

possible explicit time dependence is a COM if and only if

$$\frac{\mathrm{d}\hat{G}(t)}{\mathrm{d}t} = \frac{\partial \hat{G}(t)}{\partial t} - \frac{i}{\hbar}\left[\hat{G}(t),\, \hat{H}(t)\right] = 0, \text{ i.e.,}$$
$$\frac{\partial \hat{G}(t)}{\partial t} = \frac{i}{\hbar}\left[\hat{G}(t),\, \hat{H}(t)\right]. \tag{5}$$

Observe that an explicitly time-dependent COM *cannot* commute with the Hamiltonian. The noteworthy point is that, even in the general case in which the COM has an explicit time dependence, the corresponding unitary transformation preserves the EOM (i.e., the Schrödinger equation). That is, under the UT

$$|\Psi(t)\rangle \rightarrow |\Psi'(t)\rangle = \mathrm{e}^{-i\alpha\,\hat{G}(t)/\hbar}\,|\Psi(t)\rangle\,, \tag{6}$$

where α is time-independent, we continue to have

$$i\hbar\frac{\mathrm{d}|\Psi'(t)\rangle}{\mathrm{d}t} = \hat{H}(t)|\Psi'(t)\rangle. \tag{7}$$

It is a simple exercise to establish (4), and we invite the reader to do so. First set $|\Psi(t)\rangle = \hat{U}^{-1}(\alpha)\,|\Psi'(t)\rangle = \mathrm{e}^{i\alpha\,\hat{G}(t)/\hbar}\,|\Psi'(t)\rangle$ in (4). Note that it is the explicit t-dependence in $\hat{G}(t)$ that is to be differentiated with respect to t. We need the quantity $(\partial/\partial t)\,\mathrm{e}^{i\alpha\,\hat{G}(t)/\hbar}$. Expanding the exponential in its power series, we need $\partial\hat{G}^n/\partial t$ for all positive integer values of n. Care must be exercised, because $\hat{G}$ and $\partial\hat{G}/\partial t$ do *not* commute with each other. Hence

$$\frac{\partial \hat{G}^2}{\partial t} = \frac{\partial \hat{G}}{\partial t}\,\hat{G} + \hat{G}\,\frac{\partial \hat{G}}{\partial t} = \frac{i}{\hbar}\,[\hat{G}^2(t)\,,\,\hat{H}(t)], \tag{8}$$

using (5). Proceeding in this manner, we get

$$\frac{\partial}{\partial t}\,\hat{G}^{\,n}(t) = \frac{i}{\hbar}[\hat{G}^{\,n}(t)\,,\,\hat{H}(t)], \text{ and hence}$$
$$\frac{\partial}{\partial t}\,\mathrm{e}^{i\alpha\,\hat{G}(t)/\hbar} = \frac{i}{\hbar}\left[\mathrm{e}^{i\alpha\,\hat{G}(t)/\hbar}\,,\,\hat{H}(t)\right]. \tag{9}$$

Equation (7) then follows easily.

Note that it is the *original* Hamiltonian $\hat{H}(t)$ that appears on the right-hand side of (7). This means that solutions of the Schrödinger equation with a Hamiltonian $\hat{H}(t)$ are mapped onto other, generally different, solutions of the *same* equation by a unitary symmetry. The existence of state vectors in QM, on which UTs can act directly, is a new feature without a parallel in CM, as we shall see. This requires a deeper comparison of the two schemes.

The existence of state vectors in QM, on which unitary transformations can act directly, is a feature that has no parallel in CM.

Consider, first, the situation in CM. Recall from Part 1 that an infinitesimal CT with parameter ε and generator $G(q,p)$ implies that

$$q_r \to q_r + \varepsilon\,\{q_r\,,\,G(q,p)\}, \quad p_r \to p_r + \varepsilon\,\{p_r\,,\,G(q,p)\}. \tag{10}$$

A succession of n such infinitesimal CTs amounts, in the limit $n \to \infty$, $\varepsilon \to 0$ such that $\lim n\varepsilon = \alpha$, to a CT $C(\alpha)$ with finite parameter α. The effect of this CT on a general phase space function $f(q,p)$ can be developed step by step as follows, in terms of nested Poisson brackets:

$$f(q,p) \xrightarrow{C(\alpha)} f'(q,p) = f(q,p) + \frac{\alpha}{1!}\{G(q,p),\, f(q,p)\} + \frac{\alpha^2}{2!}\big\{G(q,p),\, \{G(q,p),\, f(q,p)\}\big\} + \ldots \tag{11}$$

The series on the right-hand side can be written in a compact form by defining the differential operator

$$\mathsf{G}(q,p) = \frac{\partial G(q,p)}{\partial q_r}\frac{\partial}{\partial p_r} - \frac{\partial G(q,p)}{\partial p_r}\frac{\partial}{\partial q_r}\,. \tag{12}$$

(As always, summation over a repeated index is to be

understood.) Then

$$f'(q,p) = f(q,p) + \frac{\alpha}{1!}\mathsf{G}(q,p)f(q,p) + \frac{\alpha^2}{2!}\mathsf{G}(q,p)\mathsf{G}(q,p)f(q,p) + \cdots = \mathrm{e}^{\alpha\,\mathsf{G}(q,p)}\, f(q,p). \quad (13)$$

Thus, from the phase space function $G(q,p)$ we construct the first-order linear partial differential operator $\mathsf{G}(q,p)$ on phase space functions; and by exponentiating this operator, we get the finite classical CT $C(\alpha)$. Symbolically,

$$C(\alpha)f(q,p) = \mathrm{e}^{\alpha\,\mathsf{G}(q,p)}\, f(q,p). \quad (14)$$

There is an analogue of the foregoing in QM, at the level of the action of UTs by conjugation on dynamical variables or operators. From (2b) we have

$$\hat{A} \xrightarrow{U(\alpha)} \hat{A}' = \hat{U}(\alpha)\,\hat{A}\,\hat{U}^{-1}(\alpha) = \mathrm{e}^{-i\,\alpha\,\hat{G}/\hbar}\,\hat{A}\,\mathrm{e}^{i\,\alpha\,\hat{G}/\hbar} = \hat{A} - \tfrac{(i\alpha/\hbar)}{1!}[\hat{G}\,,\,\hat{A}] + \tfrac{(i\alpha/\hbar)^2}{2!}\left[\hat{G}\,,\,[\hat{G}\,,\,\hat{A}\,]\right] + \ldots \quad (15)$$

In writing the last equation above, we have used Hadamard's operator identity for an expression of the form $\mathrm{e}^{-\hat{B}}\,\hat{A}\,\mathrm{e}^{\hat{B}}$, namely:

$$\mathrm{e}^{-\hat{B}}\,\hat{A}\,\mathrm{e}^{\hat{B}} = \hat{A} - [\hat{B}\,,\,\hat{A}] + \frac{1}{2!}\left[[\hat{B}\,,\,[\hat{B}\,,\,\hat{A}]\right] + \ldots\,. \quad (16)$$

As before, the nested commutators can be written in a compact form by defining an operator $\hat{\mathsf{G}}$ that acts on *operators* according to

$$\hat{\mathsf{G}}\,(\cdot) = (i\hbar)^{-1}\,[\,\hat{G},\,\cdot\,]. \quad (17)$$

Then

$$\hat{A}' = \hat{A} + \frac{\alpha}{1!}\hat{\mathsf{G}}\,\hat{A} + \frac{\alpha^2}{2!}\,\hat{\mathsf{G}}\,\hat{\mathsf{G}}\,\hat{A} + \cdots = \mathrm{e}^{\alpha\,\hat{\mathsf{G}}}\,\hat{A}. \quad (18)$$

Here, the action of taking the commutator of $\hat{G}/(i\hbar)$ with a general operator has been promoted to an operator $\hat{\mathsf{G}}$ that acts on operators themselves. Such an object is known as a super-operator or *dynamical map*. We thus have the parallel situations in classical and quantum mechanics:

- In CM: Phase space function $G(q,p) \rightarrow \mathsf{G}(q,p)$: $\mathsf{G}\, f = \{G\,,\, f\}$, any f.
- In QM: Operator $\hat{G}$ on Hilbert space $\rightarrow \hat{\mathsf{G}}$: $\hat{\mathsf{G}}\,\hat{A} = (i\hbar)^{-1}[\hat{G}\,,\, \hat{A}]$, any $\hat{A}$.

G arises from G, but the two have different mathematical natures. Similarly, $\hat{\mathsf{G}}$ arises from $\hat{G}$, and again they are different kinds of mathematical objects. The PB in G is replaced by the commutator (divided by $i\hbar$) in $\hat{\mathsf{G}}$. But the special feature of QM is the existence of state vectors $|\Psi\rangle$ on which $\hat{U}(\alpha)$ and $\hat{G}$ can act directly, in contrast to the conjugation on operators. We may say:

(i) In CM: G, the dynamical variable $\neq \mathsf{G}$, the transformation generator.

(ii) In QM: $\hat{G}$, the dynamical variable = the transformation generator, in its action on state vectors.

We can appreciate this difference in yet another way: In CM there is no significant role, and indeed generally no meaning because of dimensional reasons, for the numerical exponential expression $\mathrm{e}^{\alpha G(q,p)}$; while in QM the analogous operator expression in (1), $\hat{U}(\alpha) = \mathrm{e}^{-i\alpha\hat{G}/\hbar}$, is meaningful and important.

Reading the statement in (ii) above 'backwards', we see that in QM, operators that generate or represent transformations on state vectors are themselves observable quantities. That is why, in quantum mechanics, things like the parity transformation (or space inversion) and

Box 1. Classical-to-Quantum Correspondence: Ordering of Operators

As mentioned already, functions of the dynamical variables of a classical Hamiltonian system are replaced by operators when we go over to quantum mechanics. Unlike classical variables, these operators do not commute with each other, in general. As a result, the 'mapping' from the space of functions $f(q,p)$ to the space of operators $\hat{f}(\hat{q},\hat{p})$ is not unique, except in the simplest cases. When we attempt to replace the classical Hamiltonian $H(q,p)$ by the quantum mechanical Hamiltonian $\hat{H}(\hat{q},\hat{p})$, the order in which the operators appear in various terms of $\hat{H}$ is not uniquely specified, and this leads to ambigiuities. Up to the level of quadratic functions of the q's and p's, it is quite straightforward to make the classical variable $\rightarrow$ quantum operator correspondence, by the direct replacements $q \mapsto \hat{q}$, $p \mapsto \hat{p}$. The only non-trivial correspondence rule at this level is the replacement of the classical product $qp\,(=pq)$ by the symmetric operator combination $\frac{1}{2}(\hat{q}\hat{p}+\hat{p}\hat{q})$. But the uniqueness of the correspondence breaks down even for polynomials of order higher than the second, let alone other functions of (q,p).

A general procedure for the classical-to-quantum correspondence was first given by Weyl, and further generalized and developed by Moyal, Stratonovich, Wigner, and others. The Moyal–Stratonovich–Weyl quantization procedure enables us to start with a classical Hamiltonian system and obtain consistently the operators corresponding to arbitrary functions of the classical q's and p's in such a manner that (i) the Poisson bracket $\rightarrow$ (commutator)$/i\hbar$ requirement is satisfied, up to the leading order in $\hbar$ (see below); and (ii) a symmetry transformation acting on a classical phase space function $f(q,p)$ is implemented by a unitary transformation acting on the corresponding operator $\hat{f}(\hat{q},\hat{p})$. For our present purposes, these are the relevant properties for extending the consideration of symmetry generators in CM to the case of QM.

We mention that the quantization procedure still leaves open the question of the ordering of operators in the quantum mechanical counterpart of a classical system. More than one ordering prescription is possible. There are at least three different standard prescriptions, each leading to a specific 'quasi-probability distribution' in phase space that can be used to reproduce the quantum mechanical expectation values of any operator $\hat{f}(\hat{q},\hat{p})$ as the statistical average of the corresponding phase space function $f(q,p)$ weighted by the distribution.

Finally, for the sake of completeness, we make a comment on the inverse problem of expressing the Hilbert space formulation of quantum mechanics, involving operators and expectation values, in terms of a purely statistical description involving distribution functions in phase space. It turns out that, in order to do this consistently, and to take into account fully the non-commutativity of quantum mechanical operators, the correct replacement of the commutator (divided by $i\hbar$) is the so-called *Moyal bracket*, which is the Poisson bracket plus an infinite series of 'correction' terms involving higher derivatives with respect to the q's and p's, multiplied by powers of $\hbar$ starting with $\hbar^2$.

the operator corresponding to the permutation of identical particles are observables or dynamical variables. They obey the Heisenberg EOM, have eigenvectors and measurable eigenvalues, and so on. But this is not so at all classically: there, parity and permutation are solely rules of transformation, and are not themselves dynamical variables.

2. Lie Groups of Symmetries

Some of the foregoing comments are meant to be a comparison of the structural features of classical versus quantum mechanics. Clearly, they are not limited to our main theme, which is the connection between symmetry principles and conservation laws.

We revert now to that theme in the multi-dimensional case. A Lie group is a well-defined mathematical object, and it could be relevant in both CM and QM as a group of symmetries of some physical system or class of systems. Examples connected with space-time are the three-dimensional proper rotation group $SO(3)$, the Euclidean group $E(3)$, the Galilei group relevant to Newtonian mechanics, the proper orthochronous homogeneous Lorentz group $SO(3,1)$ of special relativity, and the Poincaré group of inhomogeneous Lorentz transformations.

We stress that one and the same group may be relevant, and be represented or expressed, in one form of mechanics or the other. Hence the group structure must go with the appropriate mechanical formalism. The situation is best conveyed by the flow chart in *Table* 1, displaying how a given group $\mathcal{G}$ of symmetries is represented classically and quantum mechanically. Let us explain the symbols and notation. Elements of the group $\mathcal{G}$ are written as $g(\boldsymbol{\alpha})$, where $\boldsymbol{\alpha} = (\alpha_1, \alpha_2, \cdots, \alpha_n)$ are the independent real parameters or coordinates that label the elements continuously and vary within their specified ranges. Here n is the order or dimension of $\mathcal{G}$, and

$\mathcal{G}:\quad g(\boldsymbol{\alpha}) = \exp(\alpha_j\, e_j),\, g(\boldsymbol{\alpha})g(\boldsymbol{\beta}) = g(\mathbf{f}(\boldsymbol{\alpha},\boldsymbol{\beta}))$ $[e_j,\, e_k] = C_{jk}{}^{l}\, e_l$	
CM	QM
$g(\boldsymbol{\alpha})$ is a CT $C(\boldsymbol{\alpha}) = \mathrm{e}^{\alpha_j\, \mathsf{G}_j}$	$g(\boldsymbol{\alpha})$ is a UT $\hat{U}(\boldsymbol{\alpha}) = \mathrm{e}^{-i\,\alpha_j\, \hat{G}_j/\hbar}$
$C(\boldsymbol{\alpha})\, C(\boldsymbol{\beta}) = C(\mathbf{f}(\boldsymbol{\alpha},\boldsymbol{\beta}))$	$\hat{U}(\boldsymbol{\alpha})\, \hat{U}(\boldsymbol{\beta}) = \mathrm{e}^{i\omega(\boldsymbol{\alpha},\boldsymbol{\beta})}\, \hat{U}(\mathbf{f}(\boldsymbol{\alpha},\boldsymbol{\beta}))$
$\Big\vert$	$\Big\vert$
$[\mathsf{G}_j, \mathsf{G}_k] = C_{jk}{}^{l}\, \mathsf{G}_l$	$[\hat{\mathsf{G}}_j, \hat{\mathsf{G}}_k] = C_{jk}{}^{l}\, \hat{\mathsf{G}}_l$
$\Big\vert$	$\Big\vert$
$\{G_j, G_k\} = C_{jk}{}^{l} G_l + d_{jk}$	$(i\hbar)^{-1}[\hat{G}_j, \hat{G}_k] = C_{jk}{}^{l} \hat{G}_l + d_{jk}$

Table 1. Pattern of classical and quantum realizations of symmetry groups.

the α_j's chosen are called *canonical coordinates of the first kind*. In the case of $SO(3)$, for instance, these are the so-called axis-angle parameters. (The Euler angles frequently used to specify rotations in three-dimensional space are *not* canonical coordinates of the first kind.) Group composition in $\mathcal{G}$ is expressed in coordinates by the n real functions $\{f_j(\boldsymbol{\alpha},\boldsymbol{\beta}),\ j = 1, 2, \ldots, n\} \equiv \mathbf{f}(\boldsymbol{\alpha},\boldsymbol{\beta})$ of $2n$ independent real arguments each. The functions $\mathbf{f}(\boldsymbol{\alpha},\boldsymbol{\beta})$ are restricted by the laws of group structure, namely: associativity, the existence of the identity element, and the existence of the inverse of every element. $\{e_j\}$ is the set of basis vectors in the Lie algebra. This is a real linear vector space whose elements describe elements in $\mathcal{G}$ that lie very close to the identity – what we have referred to (in Part 1) as 'infinitesimal transformations'. The expression of a finite group element $g(\boldsymbol{\alpha})$ in exponential form is in a sense symbolic – reminiscent of (14) and (18). The set of Lie bracket relations among the basis vectors, $[e_j,\, e_k] = C_{jk}{}^{l}\, e_l$, is a local expression of the group multiplication law. The coefficients $C_{jk}{}^{l}$ are called the *structure constants* of the Lie algebra. The quantities d_{jk} that appear in the last lines of each column are called *neutral elements*, and we shall say a little more about them shortly.

The Lie algebra corresponding to a Lie group is a real linear vector space whose elements describe those of the Lie group in the infinitesimal neighbourhood of the identity element.

Moving down along the two arms of *Table* 1, finite group elements are realized as CTs or UTs, respectively. They are 'honest' exponentials of $\alpha_j \mathsf{G}_j$ and $\alpha_j \hat{G}_j/(i\hbar)$, which represent $\alpha_j e_j$ in CM and in QM, respectively. Thanks to the commutation relations satisfied by G_j and $\hat{\mathsf{G}}_j$ in the two cases, the composition laws among CTs and UTs hold as they do in the group, apart from some phase factors in the case of UTs. (And apart, also, from certain issues related to the 'global' properties of the parameter space of the group. We do not discuss these here.) These commutation relations are concrete realizations of the abstract Lie bracket relations among the e_j's, referred to earlier. In both arms, the associative law is automatic, and does not require separate demonstration or verification.

The distinctive feature in QM is the appearance of a possible phase factor in the composition law for a unitary transformation.

The important distinctive feature in QM at the level of the composition law for the UT $\hat{U}(\boldsymbol{\alpha})$ is the appearance of the extra phase factor, $\mathrm{e}^{i\omega(\boldsymbol{\alpha},\boldsymbol{\beta})}$. Such a factor is permitted by the structure of QM, since the overall phase in a state vector $|\Psi\rangle$ is physically unobservable. It turns out that, in general, $\hbar\,\omega(\boldsymbol{\alpha},\boldsymbol{\beta})$ is an infinite series in the α_j's, β_j's and the structure constants $C_{jk}{}^{l}$, but linear in the neutral elements d_{jk}. It is straightforward to derive this result, but we shall not do so here.

When we finally descend to the last line in the two columns, we obtain PB relations among the classical COMs G_j, and commutation relations among the quantum COMs $\hat{G}_j$. In order to go from the penultimate line to the final equations in the two columns, we may either write out all the Poisson brackets (respectively, commutators) involved, and simplify the resulting expressions; or else, and less tediously, we may use the algebraic relations in (20) and (21) below, which are expressions of the *Jacobi identities* for Poisson brackets and commutators, respectively. Let f, g and h be phase space functions such that $\{f\,,\,g\} = h$. As in (12), define the

corresponding operators

$$\mathsf{f} = \frac{\partial f}{\partial q_r}\frac{\partial}{\partial p_r} - \frac{\partial f}{\partial p_r}\frac{\partial}{\partial q_r}\,, \tag{19}$$

and similarly g and h. Then the Jacobi identity for Poisson brackets translates to the commutation relation

$$[\mathsf{f}\,,\,\mathsf{g}] = \mathsf{h} \tag{20}$$

for the operators. Similarly, let $\hat{A}\,,\,\hat{B}$ be operators on a Hilbert space, and let $[\hat{A}\,,\,\hat{B}] = \hat{C}$. Further, as in the definition (17), let $\hat{\mathsf{A}} = (i\hbar)^{-1}[\hat{A}\,,\,\cdot]$ and similarly $\hat{\mathsf{B}}$, $\hat{\mathsf{C}}$ be the corresponding superoperators. Then the Jacobi identity for commutators of operators translates to the relation

$$[\hat{\mathsf{A}}\,,\,\hat{\mathsf{B}}] = (i\hbar)^{-1}\hat{\mathsf{C}} \tag{21}$$

at the level of the superoperators.

It must be noted that the final equations in both columns are stated in terms of dynamical variables. Classically, the neutral elements d_{jk} are seen only at this concluding stage, while in QM they are 'infinitesimal forms' of the phases $\omega(\boldsymbol{\alpha}, \boldsymbol{\beta})$ that have appeared earlier. (This feature again reinforces the fact that the set $\{\hat{U}(\boldsymbol{\alpha})\}$ of UTs is unique to QM, with no direct classical analogue.) There are, of course, certain functional relations these phases should satisfy, leading to conditions on the d_{jk}'s. Classically, they have vanishing PBs with all phase space functions, while quantum mechanically their commutators with all dynamical variables vanish.

In CM (respectively, QM), the neutral elements that appear in the algebra of PBs (resp., commutators) satisfied by the generators have vanishing PBs (resp., commutators) with all phase space functions (resp., operators representing dynamical variables).

At this point, we can say more precisely which quantum quantities are analogues of which classical ones, following up on our opening remarks in Section 1. To the classical CT $C(\alpha)$ there corresponds the operation $\hat{U}(\alpha)\ (\cdot\ )\ \hat{U}^{-1}(\alpha)$ of conjugation of operators in QM, rather than $\hat{U}(\alpha)$ itself. The correspondences $G \leftrightarrow \hat{G}$ and $\mathsf{G} \leftrightarrow \hat{\mathsf{G}}$ then follow. We can think of the individual factor $\hat{U}(\alpha)$ in the conjugation operation as a 'square-root' of that operation in some sense, just as the state

Box 2. A Basic Difference in the Role of Symmetry in CM and QM.

There is an important difference between CM and QM in the way a symmetry manifests itself. It is helpful to understand this difference with the help of a simple and familiar example.

Consider the Kepler problem, in which a classical particle moves in a closed orbit around a centre of force in an attractive Coulomb potential $V(r) = -\kappa/r$, where κ is a positive constant. (Recall that, in Part 1, we have discussed the COMs in this instance, including also the Laplace–Runge–Lenz vector.) The potential, and hence the Hamitonian of the particle, $H = \mathbf{p}^2/(2m) + V(r)$, are rotationally invariant – that is, H does not depend on the orientation of the coordinate axes. The particle is acted upon by a central force, so that there is no torque on it. Therefore its orbital angular momentum $\mathbf{L} = \mathbf{r} \times \mathbf{p}$ is a COM. This means that both the magnitude and the direction of $\mathbf{L}$ (and hence the plane of the orbit) remain unchanged in time as the particle traverses any orbit. But what determines $\mathbf{L}$ for any given orbit? Clearly, the initial conditions, i.e., the initial position $\mathbf{r}(0)$ and initial momentum $\mathbf{p}(0)$, do so.

Consider, for simplicity, the set of circular orbits corresponding to the set of initial conditions for which the magnitudes $r(0)$ and $p(0)$ are the same, but the vectors $\mathbf{r}(0)$ and $\mathbf{p}(0)$ point in all possible directions. The orbits in this set are circles of the same radius, but lying in all possible planes. However, a rotation of the coordinate axes will take us from any of these orbits to any other. Any particular orbit breaks the rotational invariance of the Hamiltonian, but spherical symmetry is restored in the full *set* of orbits.

In contrast, the situation in QM is quite different. All possible solutions of the Schrödinger equation that are related to each other by a symmetry transformation are *superposed* to constitute the state vector (or wave function) of the system. The quantum mechanical analogue of the classical example considered above is provided by the ground state of the electron in a hydrogen atom. This state has a spherically symmetric wave function, proportional to e^{-r/a_0}, where a_0 is the Bohr radius. Thus the ground state *retains* the property of rotational invariance that the Hamiltonian enjoys. (This feature is quite general for quantum mechanical systems, and may be termed the *Weyl–Wigner realization* of symmetry, after Hermann Weyl and Eugene Wigner.) On the other hand, note that the most probable value of r in the ground state is not zero, but rather, the Bohr radius a_0 ; and yet the orbital angular momentum quantum number of the state is $l = 0$. This is only possible because, in a sense, all possible classical orbits are *superposed* to produce the single wave function corresponding to the ground state.

vector $|\Psi\rangle$ is a (complex) 'square-root' of the probability. A single factor $\hat{U}(\alpha)$ can act on $|\Psi\rangle$. As we have reiterated, this is a uniquely quantum mechanical feature.

When the Lie group of symmetries is related to space-time transformations, the corresponding constants of the motion are important mechanical quantities such as the linear momentum, energy and angular momentum.

Some remarks on the physical meaning of the COMs G_j and $\hat{G}_j$ are in order. When the Lie group $\mathcal{G}$ is related to space-time, these COMs are important mechanical quantities. If $\mathcal{G}$ is the 3-parameter group $SO(3)$ of spatial rotations, the generators are the components of the total angular momentum of the physical system. When spatial translations are included and $\mathcal{G}$ becomes the 6-parameter Euclidean group $E(3)$, the additional generators are the components of the total linear momentum. Next, extension to the nonrelativistic Galilei group or to the relativistic Poincaré group, both of which are 10-parameter groups, brings in time translations and the three generators of pure velocity transformations (or boosts). The generator corresponding to time translations is the Hamiltonian. If the system has time-translation invariance, i.e., if the Hamiltonian H has no explicit time dependence, then H is a COM. (Its numerical value is the total energy of the system, in the usual situations.) The generators of boosts are somewhat nontrivial. The corresponding COMs are related to the motion of the centre of mass and the centre of energy, respectively, in the nonrelativistic and relativistic cases. Recall that, in Part 1, we have already illustrated how the 10 Galilean invariants of the motion arise explicitly in a system of particles interacting via 2-body potentials that depend only on the distances between pairs of particles. Each of the space-time groups listed above is in fact relevant for whole classes of physical systems.

A comment on the neutral elements d_{jk} : It so happens that, out of all the Lie groups relevant in physical contexts, the Galilei group is the only one where a nontrivial neutral element can be present, and in that case it is the total mass of the system. In all other cases – $SO(3)$, $E(3)$, and the Poincaré group – they turn out to be trivial, and can be ignored. Interestingly, in the case of Galilean quantum mechanics, the fundamental

Heisenberg canonical commutation relations turn out to be a consequence of the Lie algebra relations pertaining to the Galilei group.

Finally, let us make a few comments on the dynamical symmetry group of any given system, in order to put this aspect in perspective, and also to summarise very briefly a few key points. Discovering the COMs of a dynamical system is not a trivial task, either in CM or in QM. In CM, we need to find all phase space functions $G(q, p, t)$ such that $\mathrm{d}G/\mathrm{d}t \equiv 0$. In QM, we need to find all quantum observables $\hat{G}$ such that $\mathrm{d}\hat{G}/\mathrm{d}t \equiv 0$. All these COMs will generate symmetries of the dynamical system. It helps to note that the PB of two COMs is again a COM, even if the two COMs have explicit time dependence. (It is an instructive exercise to establish this statement, which is called Poisson's Theorem.) Likewise, in QM, the commutator of two COMs is again a COM. In each case, we must discover the largest possible group of such symmetries. This will be some subgroup of the group of CTs (in CM) or UTs (in QM) of the system.

The existence of COMs and symmetry generators is closely linked to the integrability or otherwise of the dynamical system. This is a subject by itself, and we shall not discuss it here. However, some remarks about a specific example might be useful to the reader. This is the classical Kepler problem of a nonrelativistic particle moving in an inverse-square field of force, discussed in Part 1. We saw there that the COMs generating symmetries were the Hamiltonian H (time-translation invariance), the angular momentum $\mathbf{L}$ (rotation invariance) and the Laplace–Runge–Lenz vector. The first two are somewhat obvious symmetries, because H is not explicitly time-dependent, and is clearly rotationally invariant. The existence of the Laplace–Runge–Lenz vector, however, shows that the Kepler problem truly has a further hidden symmetry. The (dynamical) symmetry

Box 3. Amalie Emmy Noether (1882–1935)

No discussion of symmetry can be complete without a special mention of the great mathematician Emmy Noether, whose seminal work on the relationship between symmetry principles and conservation laws is a central theme in modern physics. The examples we have used as illustrations in this set of articles are special cases of her fundamental theorems, which find their full expression in systems with continuously infinite numbers of degrees of freedom – namely, classical and quantum fields. The Wikipedia article on Emmy Noether gives a succinct account of the life and achievements of this extraordinary intellect. Scientists and mathematicians of the calibre of Einstein, Hilbert and Weyl have acclaimed her as the greatest woman mathematician in recorded history. Among other achievements, an entire field of modern mathematics, abstract algebra, may be said to be her creation.

group in this case is not just $SO(3)$, as it would be for a particle moving in a general spherically symmetric potential. It turns out to be a larger sub-group of the group of CTs of the system – it is $SO(4)$ in the case of an attractive r^{-1} potential. The implications of this fact are equally interesting in the quantum-mechanical counterpart of the problem, namely, the (nonrelativistic) electron in a hydrogen atom. Symmetry, in general, implies degeneracy of the spectrum of the Hamiltonian, i.e., of the energy levels. For a particle in a general spherically symmetric potential, rotational invariance implies that the energy levels cannot depend on the 'magnetic' quantum number m. In the case of an attractive r^{-1} potential, they do not depend on the orbital angular momentum quantum number l, either. The energy levels E_n of the electron in a hydrogen atom depend only on the principal quantum number n. This absence of any dependence of E_n on l is familiar to you as *accidental degeneracy*. Its origin actually lies in the extra dynamical symmetry of this system.

Symmetry, in general, implies degeneracy of the energy levels of a quantum mechanical system.

3. Broken Symmetry

Our pedagogical account of the way continuous symmetries of dynamical systems are connected to conservation laws will hopefully convince the reader that this is a very important and beautiful component of both classical mechanics and quantum mechanics. The ideas of

symmetry transformations, action principles, generators and COMs mesh together so intricately in the classical Hamiltonian and the quantum operator formalisms. One aspect of CM which should also be looked at in this context is the Hamilton–Jacobi formulation which stands, in some sense, at the same level as the state vector or wave function in QM. But this formulation must be given a character that is globally well-defined in the phase space concerned. Proper implementation of this task requires a combination of ideas from symplectic and differential geometry. We have therefore not ventured into it here.

In systems with an infinite number of degrees of freedom, a different and more subtle realization of symmetry is possible, that is absent in systems with a finite number of degrees of freedom.

There is, however, another very important aspect of symmetry that is so fundamental in nature that it deserves at least a mention in this article. As mentioned at the outset in Part 1, our discussion, though restricted to systems with a finite number of degrees of freedom (NDF), can be generalized to systems with an infinite NDF. Two types of physical systems are of interest in this regard: (i) Macroscopic collections of interacting particles, studied in statistical mechanics; in the so-called thermodynamic limit, the number N of particles and the volume V of the system both tend to infinity such that their ratio remains finite. (ii) Fields of different kinds, for which the NDF is a continuous infinity – one or more degrees of freedom being associated with each point in space. In the context of symmetry, a very interesting and important new feature arises in such systems. This feature is absent in the case of systems with a finite NDF.

As mentioned in *Box* 2, the standard manner in which symmetry is manifested in QM is the Weyl–Wigner realization. The ground state of a system possesses the symmetry of the Hamiltonian. In systems with an infinite NDF, however, there is another, more subtle realization of symmetry that may be termed the *Nambu–Goldstone realization*, after Yoichiro Nambu and Jeffrey Goldstone.

'Spontaneous symmetry breaking' is something of a misnomer, because there is really no breakdown of symmetry, but merely a less obvious realization of it.

In this case, the system has a whole *set* of possible ground states, such that we can go from one ground state to another by a symmetry transformation (a transformation that keeps the Hamiltonian unchanged). The system selects one of this set of ground states – either randomly, triggered by fluctuations, or as a result of the manner in which it is prepared. An individual ground state does *not* possess the symmetry of the Hamiltonian. On the other hand, the *set* of possible ground states does have this symmetry. Moreover, there are certain collective excitations of the system (called Goldstone bosons) that connect the different possible ground states, and thus help restore the symmetry broken by the choice of a specific ground state. This is the phenomenon known as the *spontaneous breakdown of symmetry*. This phrase is something of a misnomer, because there is really no breakdown of symmetry, merely a different and less obvious realization of it. The term *secret symmetry* is also used in this context, but 'spontaneous breakdown of symmetry' is the more common name for the phenomenon.

An example from condensed matter physics is helpful in understanding the issue. Among other effects, the spontaneous breakdown of symmetry plays a crucial role in certain phase transitions in condensed matter. Consider a ferromagnetic material. We are concerned with a system at a non-zero temperature. Hence it is the free energy (rather than the Hamiltonian itself), and the thermodynamic equilibrium state (rather than the ground state) of the system, whose symmetry we have to consider. The equilibrium state of the material is effectively represented by its remnant or 'spontaneous' magnetization $\mathbf{M}_0$. (The subscript serves to remind us that this is the magnetization in the absence of a magnetic field.) At any temperature above the Curie temperature of the material, the different atomic magnetic dipole moments (equivalently, spins) are disordered, and the net magne-

tization $\mathbf{M}_0 = 0$. The interaction between these spins is invariant under rotations of the coordinate axes. Thus both the free energy and the magnetization (the counterparts of H and the ground state) share the property of rotational symmetry. (The null vector is rotationally invariant!) This is the situation in the so-called disordered or paramagnetic phase of the material.

When the temperature of the material is lowered to a value below the Curie temperature, the material goes into its ordered or ferromagnetic phase. It acquires a non-zero magnetization $\mathbf{M}_0$. The equilibrium state of the material no longer has the rotational symmetry of the free energy, since the direction of $\mathbf{M}_0$ singles out a special direction in space. The actual direction in which $\mathbf{M}_0$ points is arbitrary, and may be selected in practice by placing the material in a small applied magnetic field in any desired direction, cooling the sample to below its Curie temperature, and then switching off the field. States corresponding to different possible directions of $\mathbf{M}_0$ are connected by collective excitations known as spin waves, which are the Goldstone bosons in this instance.

Where does the condition of an infinite NDF come in? It turns out that there can be no spontaneous breakdown of symmetry in a system with a finite NDF because of the internal or intrinsic *fluctuations* in the system. Now, there are two primary, distinct, sources of such fluctuations in nature: quantum fluctuations (owing to the fact that $\hbar \neq 0$), and thermal fluctuations (at any non-zero temperature). They have, in general, the effect of restoring the symmetry of the state of the system. A simple example is provided by a particle moving in one spatial dimension, under the influence of the symmetric double-well potential $V(x) = k(x^2 - a^2)^2$, where k and a are positive constants. The Hamiltonian of the particle is invariant under the reflection (or, in this case, parity) transformation $x \mapsto -x$. The points $x = \pm a$ are minima of the potential. A classical particle in this potential

There can be no spontaneous breakdown of symmetry in a system with a finite number of degrees of freedom because of the internal fluctuations (both thermal and quantum) in the system.

The occurrence of spontaneous symmetry breaking depends on a rather small number of basic features. It is the mechanism underlying phase transitions in a large number of physical systems, from superconductors to the quark-gluon plasma.

has two stable equilibrium states of minimum energy: $(x, p) = (a, 0)$ and $(x, p) = (-a, 0)$. When it is in either of these two states, it breaks the reflection symmetry of the Hamiltonian, although the *pair* of equilibrium states does have that symmetry. Now consider what happens in QM, where the particle can *tunnel* from one well of the potential to the other. The true ground state of the particle has a wave function that is symmetric under $x \mapsto -x$, with maxima of equal heights at $x = \pm a$ and a minimum at $x = 0$. Thus, quantum fluctuations (tunnelling being one manifestation of these) lead to a ground state that has the same symmetry property as the Hamiltonian, in this case. More generally, quantum fluctuations, or thermal fluctuations, or a combination of both, ensure that the ground state (or equilibrium state) of any system with a finite NDF has the same symmetry as its Hamiltonian.

Only when the NDF is *infinite* is there a possibility of genuine spontaneous breakdown of symmetry, under suitable conditions. These conditions must ensure that phenomena such as tunnelling, or other effects of the intrinsic fluctuations in the system, do not suffice to restore the symmetry of the ground state or thermal equilibrium state. Take, for instance, the double-well potential example above. Imagine a lattice of such potentials, and a collection of particles in them. The probability of *coherent* or simultaneous tunnelling of all the particles may well vanish in the thermodynamic limit, as it would involve (in the lowest approximation) a product of N 'Gamow factors' or negative exponentials representing individual tunnelling probabilities, each less than unity. On the other hand, if the system is at a sufficiently high temperature, the symmetry might well be restored by thermal fluctuations. This is, of course, only a rough example, and we have not mentioned other important factors. In practice, the occurrence or otherwise of the spontaneous breakdown of symmetry depends on

a rather small number of basic features. These include the precise nature of the symmetry (e.g., discrete versus continuous symmetry), the spatial dimensionality of the system, the number of components of the physical quantity characterizing the system (such as the vector $\mathbf{M}_0$ in the magnet example above), etc.

The spontaneous breakdown of symmetry is the mechanism underlying a large number of phase transitions in a wide variety of physical circumstances, ranging from superconductors to the quark-gluon plasma in the early universe. The fact that only a few general features control the occurrence of the phenomenon leads to the famous *universality* properties associated with critical phenomena. Even at the absolute zero of temperature, when thermal fluctations are absent, there can be spontaneous breakdown of symmetry in certain systems – quantum fluctuations alone cannot restore the symmetry in such cases. This is what happens in some of the so-called *quantum phase transitions* that are of much current interest in condensed matter physics.

Suggested Reading

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Address for Correspondence

K S Mallesh[1]
Department of Studies in Physics
University of Mysore
Manasagangotri
Mysore 570 006

S Chaturvedi[2]
School of Physics
University of Hyderabad
Hyderabad 500 046

V Balakrishnan[3]
Department of Physics
Indian Institute of Technology
Madras, Chennai 600 036

R Simon[4]
The Institute of Mathematical Sciences, CIT Campus
Chennai 600 113.

N Mukunda[5]
Centre for High Energy Physics
Indian Institute of Science
Bangalore 560 012.

Email:
[1] mallesh@physics.uni-mysore. ac.in
[2] scsp@uohyd.ernet.in
[3] vbalki@physics.iitm.ac.in
[4] simon@imsc.res.in
[5] nmukunda@gmail.com