

ON THE CONNECTION BETWEEN CONSTANTS OF THE MOTION OF DIFFERENT QUANTAL SYSTEMS*

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ABSTRACT:

Quantum mechanical constants of the motion, Q , are defined as local invariants of a quantal equation of motion. They are inherently more general objects than the invariants envisaged in the Lie-Ovsjannikoy theory of the symmetry of differential equations. It is shown that for a large and important class of Schroedinger Hamiltonians H_0 and $H(\lambda)$, λ a parameter, there is a continuous one to one correspondence between the constants of the motion Q_{i0} and $Q_i(\lambda)$ for all finite times. The quantal analog of the discontinuities that Poincaré found in classical first integrals of the n -body problem are isolated and obviated. The concepts of "approximate constant of the motion" and "approximate invariant of a Schroedinger equation" can thus be usefully defined and the algebraic properties of perturbed systems related to those of the unperturbed system.

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1. INTRODUCTION

Sophus Lie based his group theoretical treatment of systems of differential equations¹

$$F^r(x, u, \partial_j u, \partial_j \partial_k u \dots) = 0; \quad r = 1, 2, \dots R \quad (1.1)$$

upon the concept of an infinitesimal transformation of a manifold

$$(x, u) \rightarrow (\bar{x}, \bar{u}) \quad (1.2)$$

with coordinates of two types

$$\begin{aligned} x &= (x^1, x^2, \dots x^n), \\ u &= (u^1, u^2, \dots u^m), \end{aligned} \quad (1.3)$$

where the u^j are considered to become functions of the x^k by virtue of the fact that (1.1) is assumed soluble.

The functions u may be taken to be the original unknown functions appearing in the set, or they may be new functions that have arisen in the reduction of the set to a new set of first-order equations through the device of introducing unknown functions for various derivatives appearing in the original set. Lie's infinitesimal transformations are of the form

$$\begin{aligned} \bar{x}^i &= f^i(x, u, \delta a), \text{ with } x^i = f^i(x, u, 0), \\ \bar{u}^j &= g^j(x, u, \delta a), \text{ with } u^j = g^j(x, u, 0). \end{aligned} \quad (1.4)$$

Using such transformations and their first extensions² Lie gave a definitive treatment of the continuous symmetries of finite sets of first order ordinary differential equations. It is upon this foundation that the theory of the canonical transformation of Hamilton's equations has been erected.

Ovsjannikov has extended Lie's treatment to sets of partial differential

equations,³ but though the transformations he allows are adequate for many purposes, they are not sufficiently general to deal with the local symmetries of the partial differential equations of Schroedinger.⁴

It is not in general possible to use Lie's methods to find the symmetries of a classical system and obtain those for its quantum mechanical counterpart by replacing the momenta by differential operators. It is well known that this leads to ambiguities in all but the simplest cases.

To treat the local symmetries of Schroedinger equations one must in fact allow transformations of the form⁴

$$\begin{aligned} x^i &= f^i(x, u, \partial_j u, \partial_j \partial_k u \dots; \delta a) , \\ u^j &= g^j(x, u, \partial_j u, \partial_j \partial_k u \dots; \delta a) , \end{aligned} \tag{1.5}$$

and make no *a priori* restrictions upon the maximum order of derivative that can appear in the transformation.

We have used transformations of the form (1.5) to obtain the generators of the groups of a variety of time-dependent Schroedinger equations.⁴⁻⁷ Each such transformation can be considered to be brought about by a linear differential operator Q . If;

$$(H - i\partial_t) \Psi(x, t) = 0 , \tag{1.6a}$$

the operators Q satisfy

$$(H - i\partial_t) Q\Psi(x, t) = 0 , \tag{1.6b}$$

for all Ψ satisfying (1.6a). From this it follows that

$$\{ \partial_t Q + i [H, Q] \} \Psi = 0 , \tag{1.7}$$

and that

$$(d/dt) \langle \Psi_j | Q | \Psi_k \rangle = 0 , \tag{1.8}$$

for all Ψ_j and Ψ_k satisfying (1.6a).

These operators are thus the quantum mechanical analogs of classical constants of the motion.⁸ Each local symmetry is seen to give rise to a conserved quantity, and every function of an operator Q which is well defined on the space of states of the system is the operator representative of a corresponding conserved quantity.

It of course does not follow that every such Q is the generator of a finite dimensional Lie group. Some of the operators are generators of the geometrical symmetry group (degeneracy group) of the Hamiltonian. These are the explicitly time-independent operators that commute with the Hamiltonian. Some of the Q 's are generators of what have been termed "dynamical groups", others are not. Some of the operators are functions of others directly, while some become so, only by virtue of identities implied by the Schroedinger equation.

In fact, once one has found a set of Q 's which contains for each degree of freedom k , a pair of invariants such that

$$\begin{aligned} [Q_{x^k}, Q_{p_l}] &= i\delta_l^k, \\ [Q_{x^k}, Q_{x^l}] &= 0, \\ [Q_{p_k}, Q_{p_l}] &= 0, \end{aligned} \tag{1.9}$$

then one has available a complete set of generators for the Heisenberg algebra and Weyl group of the system.* With these one can construct generators of a tremendous variety of further Lie algebras and Lie groups. It is thus difficult to define what one means by a "maximal" invariance group of a differential equation, or by a "minimal" group unless one puts restrictions upon the form of the generators or the algebra or group.

Because of the usefulness of constants of the motion it is unfortunate that the generality of the transformation (1.5) makes it difficult in practice to find interesting local symmetries of even quite simple Schroedinger equations. It would therefore be most helpful to have methods for relating the local symmetries of a complex system to those of a simpler system, and methods for finding "approximate" symmetries. However, one might anticipate that even in principle this is a non-trivial problem.

*The time is being considered a parameter rather than a dynamical variable.

In classical mechanics the problem of relating the constants of the motion of one system to those of another has been known to present some very troublesome features.

In 1892 Poincaré's famous theorem on the nonexistence of uniform integrals of motion for the n -body problem was published in his "Methodes Nouvelles de la Mechanique Celeste".⁹ Poincaré considered bound conservative systems obeying the equivalent of Hamiltonians equations

$$\dot{p}_j = -\partial H / \partial q^j; \quad \dot{q}^j = \partial H / \partial p_j \tag{1.10}$$

and supposed

$$H = H_0 + \mu H_1 + \mu^2 H_2 + \dots, \tag{1.11}$$

with

$$H_0 = H_0(p_1, p_2 \dots), \quad H_i = H_i(p_1, p_2 \dots; q^1, q^2 \dots), \quad i > 0, \tag{1.12}$$

as happens when the p 's are the action variables obtained via a Hamilton-Jacobi treatment of H_0 . Supposing $I(\mu; p_1, p_2 \dots; q^1, q^2 \dots)$, to be a first integral of system (1.10) to (1.12), so that

$$[H, I]_{PB} = 0, \tag{1.13}$$

he showed that for $n > 2$, I cannot in general be analytic and uniform for all real values of the q^j , for small values of μ , and for values of the p_j in an arbitrary and arbitrarily small domain. In particular I can not be developed in a power series in μ of the form

$$I = I_0 + \mu I_1 + \mu^2 I_2 + \dots, \tag{1.14}$$

such that $I_0, I_1, I_2 \dots$ are uniform in the p_j and q^j , and periodic in the individual q^j .

Since the p_j of a Hamilton-Jacobi treatment satisfy (1.13) for $H = H_0$

and otherwise, Poincaré's proof also shows that the corresponding action variables are not, for the general H of (1.11), uniform functions of the variables of the unperturbed problem. The argument of Poincaré fails when applied to second integrals, and so far as we are aware a corresponding theorem has neither been proved nor disproved for them.

Perusal of Poincaré's proof shows that it is the existence of resonances (in the classical-mechanical sense) that is central to the pathological behaviour that he finds. Brillouin gave an extensive discussion of this point and showed by example that the discontinuities can occur in dissipative systems as well.¹⁰

Poincaré's theorem followed closely upon the work of Bruns who showed in 1887 that the seven classical integrals of energy, linear, and angular momentum are the only independent integrals of the three-body problem that are algebraic functions of the positions, momenta, and time.¹¹ Painlevé extended Bruns theorem in 1898 by showing that every integral of the n -body problem that is an algebraic function of the velocities is a function of the seven classical integrals only.¹²

Each of the theorems recounted here admits of exceptions, and those which are relevant to problems of celestial mechanics were dealt with by their authors. Further exceptions exist for special systems, such as coupled oscillators, so that the theorems must not be applied uncritically.

Nevertheless Poincaré's theorem is particularly sobering. If his discontinuities persist in quantum mechanics and cannot be gotten around, then whenever one attempts to relate the invariants of an n -body system to those of a simpler unperturbed system; one must envisage the use of the theory of singular perturbations. Perhaps the happiest statement one can make about such a situation is that quantum mechanics could then enshrine many otherwise impossible surprises.

2. QUANTAL FIRST INTEGRALS

To determine the effect of changes in a Hamiltonian $H(\mu)$ upon explicitly time-independent constants of the motion in the Schroedinger picture we require in this section that

$$[H(\mu), Y] \Psi = 0 \quad (2.1a)$$

if

$$H(\mu) \Psi(\mu) = E(\mu) \Psi(\mu) \quad (2.1b)$$

Because Y satisfies (2-1) it in general becomes a function of μ and we wish to determine whether this functional dependence is a continuous one. We shall suppose that the system is confined to a box of large but finite size, so that the Hamiltonian has a discrete spectrum over the entire range of μ of interest. Let $H(\mu_0)$ be defined by its matrix representation $\underline{H}(\mu_0)$ on the basis of its eigenfunctions. In this representation we shall suppose that $\underline{H}(\mu_0 + \delta\mu)$ is a bounded operator not equal to $\underline{H}(\mu_0)$, and continuously connected to $\underline{H}(\mu_0)$:

$$\lim_{\delta\mu \rightarrow 0} \underline{H}(\mu_0 + \delta\mu) = \underline{H}(\mu_0) \quad (2.2)$$

As $\underline{H}(\mu_0)$ is a diagonal matrix, a typical element of its commutator with an arbitrary matrix \underline{X} is

$$[\underline{H}(\mu_0), \underline{X}]_{ij} = X_{ij} (\underline{H}(\mu_0)_{ii} - \underline{H}(\mu_0)_{jj}) \quad (2.3)$$

Thus if \underline{X} is to commute with $\underline{H}(\mu_0)$ and so become a first integral $\underline{Y}(\mu_0)$ it is necessary that either $X_{ij} = 0, i \neq j$, or that $H(\mu_0)_{ii} - H(\mu_0)_{jj} = 0$. That is, all off-diagonal elements of X must vanish except those that effect a mixing of degenerate states. In all other respects the elements of \underline{X} are arbitrary.

If $\underline{H}(\mu_0)$ is an $N \times N$ matrix and it has degenerate submatrices of dimension $n_1 \times n_1, n_2 \times n_2 \dots$ with $\sum n_i = N$, then there are $M = \sum n_i^2$ independent elements in a matrix $\underline{Y}(\mu_0)$ that commutes with it. From this it follows that there are M linearly independent first integrals, which we will denote \underline{Y}^i . We may choose these to be linear combinations of matrices \underline{A}^{kl} whose sole non-vanishing element is a 1 at the intersection of row k and column l such that $E_k = E_l$. Then $\underline{Y}^i = y_{kl}^i \underline{A}^{kl}$. The \underline{A}^{kl} satisfy the commutation relations

$$[\underline{A}^{kl}, \underline{A}^{rs}] = \underline{A}^{ks} \delta_{lr} - \underline{A}^{rl} \delta_{ks} \quad (2.4)$$

and together generate the group

$$U(n_1) \times U(n_2) \dots \tag{2.5}$$

This is a degeneracy group of the system.

If the perturbation engendered by letting $\mu_0 \rightarrow \mu_0 + \delta\mu$ lifts the degeneracies in one or more of the submatrices of $\underline{H}(\mu_0)$ then the original arbitrariness of the off-diagonal elements of $\underline{Y}^i(\mu_0)$ is removed if $\underline{Y}^i(\mu_0 + \delta\mu)$ is to commute with $\underline{H}(\mu_0 + \delta\mu)$. These off-diagonal elements must become zero no matter how small the perturbation and remain zero for some non-trivial range of μ . Consequently, they must in general undergo a discontinuous change as $\mu_0 \rightarrow \mu + \delta\mu$. If the change in parameter produces new degeneracies then there are also matrix elements in \underline{Y}^i that become freely variable as $\underline{Y}^i(\mu_0) \rightarrow \underline{Y}^i(\mu_0 + \delta\mu)$, though they had to be zero in $\underline{Y}(\mu_0)$. Thus, in general, \underline{Y}^i undergoes a discontinuous change as the Hamiltonian changes continuously. Furthermore the group $U(n_1) \times U(n_2) \dots$ changes discontinuously to $U(n_1)' \times U(n_2)' \dots$

The generators \underline{A}^{kl} in the eigenrepresentation of $\underline{H}(\mu_0)$ may provide the operator basis for representations of other groups. Commonly one is interested in groups such as $O(3)$ and $O(4)$ that are degeneracy groups no matter what the size of the basis. Thus if one were to diagonalize the energy matrix for the hydrogen atom one would find the invariance group $U(1) \times U(4) \times U(9) \dots$ corresponding to the n^2 fold degeneracy of the n -th energy level. However the eigenrepresentation provides a basis not only for the defining representation of this group, but also for a direct sum of the 1, 4, 9 ... dimensional representations of $O(4)$. Let $\underline{J}(\mu_0)$ be the matrix representation of a generator J of such a group on the eigenbasis of $H(\mu_0)$. Then we may write

$$\underline{J} = J_{rs} \underline{A}^{rs} \tag{2.6}$$

where

$$J_{rs} = \langle \Psi_r(\mu_0) | J | \Psi_s(\mu_0) \rangle \tag{2.7}$$

If as $\mu_0 \rightarrow \mu_0 + \delta\mu$ any degeneracy $E_k = E_l$ is lifted and $J_{kl}(\mu_0) \neq 0$, then \underline{J} suddenly ceases to commute with \underline{H} ; the \underline{J} 's themselves in general inherit the same kind of discontinuous behaviour as do the \underline{Y} 's. Contrariwise, if for some \underline{J} the $J_{kl}(\mu_0) = 0$ for all levels k, l whose degeneracy is lifted, then the \underline{J} remains a constant of the motion. In general however, the quantal first integrals and degeneracy groups of the perturbed and unperturbed Hamiltonian are not continuously connected.

If we remove our system from its container it becomes possible for discrete spectra to become continuous, and vice versa, as well as for spectral concentration points to develop and disappear. Under these conditions it is sometimes possible for a first integral of one system to change continuously into a quite different first integral of another, though this is by no means a common occurrence. However an example is provided by the Hamilton-Runge-Lenz vector of Keplerian systems

$$A = (-2H(Z))^{-\frac{1}{2}} \left\{ \frac{1}{2}(\mathbf{L} \times \mathbf{p} - \mathbf{p} \times \mathbf{L}) + Z \hat{\mathbf{r}} \right\}$$

which, as $Z \rightarrow 0$, changes continuously into a first integral of the resulting free-particle Hamiltonian $H(0)$. Poincaré's theorem tells us not to expect this to happen when three or more bodies are involved in the system of interest.

3. JOINT TRANSFORMATION OF TIME-DEPENDENT AND TIME-INDEPENDENT INVARIANTS

Let H_a be the Schroedinger Hamiltonian of an n -particle system and let it be self adjoint on the Hilbert space $\mathcal{H} = \mathcal{L}^2(R^{3n})$ of functions $\phi(x)$, $x = (x_1 \dots x_{3n})$, with scalar product

$$(\phi', \phi) = \int d^{3n}x \phi'(x)^* \phi(x) . \tag{3.1}$$

Let the time evolution operator S be defined by the usual Dunford-Taylor integral¹³

$$S \equiv \exp(+iHt) \stackrel{\text{def}}{=} (2\pi i)^{-1} \int_{\Gamma} dy \exp(yt) (y - iH)^{-1} . \tag{3.2}$$

Then

$$(H_a - i\partial_t) \Psi_a(\vec{x}, t) = 0 \tag{3.3}$$

for all

$$\Psi_a(x, t) = \{ \exp(-iHt) \} \phi(x) = S_a^{-1} \phi(x) \tag{3.4}$$

for all $\phi \in \mathcal{D}(H_a)^*$

Let Q_a be an invariant of H_a so that

$$\{ \partial_t Q_a + i [H_a, Q_a] \} S_a^{-1} \phi = 0 \tag{3.5}$$

for all ϕ , and let Q_a be self adjoint in \mathcal{H} with $\mathcal{D}(Q_a) \equiv \mathcal{R}(Q_a) \equiv \mathcal{D}(H_a) \equiv \mathcal{R}(H_a)$ so that Q_a is the operator corresponding to an observable, and Q_a and $H_a - i\partial_t$ are simultaneously diagonalizable. Then by the Stone-von Neumann operator calculus¹⁴ $\exp iH_a t$ is a unitary operator for all finite t , and Q_a , the Heisenberg representation of Q_a exists for all finite t , is self-adjoint,¹⁵ and is given by

$$Q_a = S_a Q_a S_a^{-1} \tag{3.6}$$

Now let the H_b be the Schroedinger Hamiltonian of another system b involving the same degrees of freedom as H_a , and let H_b be self-adjoint on the same Hilbert space as H_a . Then

$$(H_b - i\partial_t) \Psi_b(x, t) = 0, \tag{3.7}$$

if

$$\Psi_b(x, t) = \{ \exp -iH_b t \} \phi(x), \tag{3.8}$$

and $\phi \in \mathcal{D}(H_b)$.

Furthermore the Schroedinger operator

$$Q_{ab} = \{ \exp -iH_b t \} \tilde{Q}_a \{ \exp iH_b t \} \tag{3.9}$$

exists for all finite t .

Now one has formally

* $\mathcal{D}(G)$ signifies the domain of the operator G , $\mathcal{R}(G)$ its range.

$$S_b(\partial_t Q_{ab}) S_b^{-1} = S_b(-i[H_b, Q_{ab}]) S_b^{-1} + S_b\{S_b^{-1}S_a(i[H_a, Q_a] + \partial_t Q_a) S_a^{-1} S_b\} S_b^{-1} \quad (3.10)$$

and rigorously, for all $\phi \in \mathcal{D}(H_a)$,

$$S_b\{\partial_t Q_{ab} + i[H_b, Q_{ab}]\} S_b^{-1}\phi = S_a\{\partial_t Q_a + i[H_a, Q_a]\} S_a^{-1}\phi. \quad (3.11)$$

If $\mathcal{D}(Q_{ab}) \equiv \mathcal{R}(Q_{ab}) \equiv \mathcal{D}(H_b) \equiv \mathcal{R}(H_b)$, then for all finite t , Q_{ab} is a constant of the motion of system b , and we have established a one-to-one correspondence between constants of the motion of H_a and those of H_b . As

$$Q_{ab} = S_b^{-1}S_a Q_a S_a^{-1} S_b, \quad (3.12)$$

time-independent invariants (first integrals) may be converted to time-dependent invariants (second integrals) and vice versa.

This transformation of a constant of the motion of one system into that of another is perhaps most simply exemplified by the case where the systems are two-dimensional isotropic and anisotropic oscillators respectively. The isotropic oscillator has the first integral of angular momentum,

$$L_z = xp_y - yp_x, \quad (3.13)$$

as one of the eight generators of its dynamical group $SU(2, 1)$. The corresponding generator for the anisotropic oscillator is (L_z commutes with H_a):

$$Q_{ab} = \bar{L}_z = \{\exp -iH_b t\} L_z \{\exp iH_b t\}. \quad (3.14)$$

The matrix elements of L_z on the basis $\exp -iH_b t\phi$ are given by

$$\langle \phi S_b | S_b^{-1} L_z S_b | S_b^{-1} \phi \rangle = \langle \phi | L_z | \phi \rangle. \quad (3.15)$$

It is evident that though \bar{L}_z is an explicit function of the time, its matrix elements in this basis are constant. The matrix elements on the basis of eigenstates of H_b may be written

$$\langle \phi_b | S_b | S_b^{-1} L_z S_b | S_b^{-1} \phi_b \rangle = \langle \phi_b | L_z | \phi_b \rangle . \quad (3.16)$$

They may be evaluated by expressing $\phi_b(x)$ as a superposition of functions $\phi_a(x)$, the eigenfunctions of \tilde{H}_a . As this is a clearly convergent process these matrix elements are well defined.

As another example we consider the behaviour of a time-dependent constant of the motion when a Hamiltonian is changed. The classical free particle possesses the second integral

$$x_0 = x - (p/m) t , \quad (3.17)$$

as does the corresponding quantum mechanical system.¹⁶ Let us set $m = 1$ and consider the change from a free particle system a to a harmonic oscillator system with force constant k . Then

$$S_a = \exp \frac{1}{2} i p^2 t , \quad S_b = \exp \frac{1}{2} i (p^2 + k x^2) t , \quad S_a x_0 S_a^{-1} = x \quad (3.18)$$

This gives rise to the harmonic oscillator invariant¹⁶

$$S_b^{-1} x S_b = x \cos k^{\frac{1}{2}} t - k^{-\frac{1}{2}} p \sin k^{\frac{1}{2}} t . \quad (3.19)$$

It is a linear combination of the generators of $SU(1, 1)$ that shift the oscillator level by one unit. In this example it is not possible to choose the states ϕ to be free particle eigenstates in the Heisenberg representation, viz., $(2\pi)^{-\frac{1}{2}} \exp i\rho x$, as these are not members of a Hilbert space. However, a complete set of wave packets may be chosen instead.

Let us now consider the question of whether the correspondence between the Q_{ab} and Q_a is a continuous one when H_a and H_b are continuously connected. Let $H = H_a + \lambda V$. H_b will certainly be self-adjoint on the same Hilbert space as H_a if H_b is relatively bounded with respect H_a , with H_a bound less than 1.¹⁷ Furthermore, whenever H_a and H_b are self adjoint on the same Hilbert space, S_b strongly converges to S_a as $\lambda \rightarrow 0$, i. e.

$$\{ \exp i(H_a + \lambda V) t \} \phi \rightarrow \{ \exp iH_a t \} \phi \text{ as } \lambda \rightarrow 0 \text{ for } \phi \in \mathcal{H}, . \quad (3.20)$$

and it does so uniformly for all finite t .¹⁸ Consequently

$$Q_{ab}(\lambda) \phi \rightarrow Q_a \phi \quad (3.21).$$

in the same manner, as $\lambda \rightarrow 0$. Hence in both this sense and in the sense of weak convergence, Q_{ab} is continuously connected to Q_a under the hypothesis made.

As an example of the theorem, one may let H_a be the kinetic energy operator of n particles, and let

$$V = \sum_{j=1}^n (e_j/r_j) + \sum_{j < k} (e_{jk}/r_{jk}) \quad (3.22)$$

with $0 \leq \lambda \leq 1$, so that H_b represents the Hamiltonian of a coulombic system, while H_a is that of a system of free particles. Kato has shown that for this case H_b is H_a bounded with relative bound zero.¹⁹ The constants of the motion of the interacting system are thus continuously connected to those of the free-particle system.

It is important to note that we have in this section, as contrasted with section 2, freed ourselves from reference to a particular basis, e. g., an eigenbasis of H_a . This has made it possible to eliminate from consideration the discontinuous change in basis that would in general occur if one insisted upon referring each operator $Q(\lambda)$ to an eigenbasis of $H_b(\lambda)$, (whenever the variation in λ lead to a destruction of degeneracies or spectral concentration points). In the usual perturbation theories one implicitly or explicitly seeks to establish three types of analytic connections between their eigenvalues, and between their eigenfunctions. We here need only the analyticity of the Hamiltonians $H(\lambda)$ and the operators $Q(\lambda)$ in the sense that they are well defined self-adjoint operators. To see that this freedom is important and that there is really a hierarchy of conditions here, consider the previous examples: The eigenfunctions of an anisotropic oscillator are not in general analytically connected to those of the isotropic oscillator. There is no analytic connection between the spectrum of a harmonic oscillator and that of a free particle. The Hamiltonian operators of an atomic system and of a system of free particles are both unbounded from above. Yet in each case we have been able to establish analytic connections between the constants of the motion of the systems.

4. CONCLUSION: APPROXIMATE CONSTANTS OF THE MOTION

In the previous section we have established a continuous connection between $Q(\lambda)$, in the sense of strong convergence, and hence also in the sense of weak convergence. It is not possible to do this for first or second integrals separately. It is also not possible if one considers only invariants of the Lie-Osvjannikov type. It is only by allowing quantum mechanical constants of the motion to be unrestricted functions of the position and momentum operators, as well as explicit functions of the time, that one can obviate the difficulty unearthed by Poincaré.

In classical mechanics it may often be considered that a function $W(p, q, t)$ is a good approximate constant of the motion during the time interval $t_0 \leq t \leq t_1$ if

$$\left| (t_1 - t_0)^{-1} \int_{t_0}^{t_1} dt (dW/dt) \right| < \epsilon$$

where ϵ is a quantity that is small in some useful sense. This is a generalization of the more straightforward requirement $|dW/dt| < \epsilon$ and is useful when one wishes to separate secular from non-secular effects. We shall adopt a similar definition for an approximate constant of the motion of a system with Hamiltonian H by defining W to be a good constant of the motion on the manifold of states $\Psi = S\xi$, $\xi \in \mathcal{H}$, during the time interval $t_0 \leq t \leq t_1$, if

$$\left| (t_1 - t_0)^{-1} \int_{t_0}^{t_1} dt \langle \xi' | S(dW/dt) S^{-1} | \xi \rangle \right| < \epsilon .$$

We have seen that for an n -body system with Hamiltonian $H_b(\lambda) = H_a + \lambda V$, only constants of the motion that are allowed to take on an explicit time dependence can in general be expanded in power series about $\lambda = 0$. It is thus important to allow approximate first integrals to be objects that may have an explicit, though weak, time dependence. As

$$i[H, W] S^{-1} \phi = (dW/dt) S^{-1} \phi - (\partial W / \partial t) S^{-1} \phi ,$$

we define W to be a good approximate quantal first integral on the manifold

of functions $\xi \in \mathcal{H}$ during the time interval $t_0 \leq t \leq t_1$ iff

$$\left| (t_1 - t_0)^{-1} \int_{t_0}^{t_1} dt \langle \xi' | S_i [H, W] S^{-1} | \xi \rangle \right| < \epsilon .$$

With this definition W need not be an exact second integral to qualify as an approximate first integral. However, we can ensure that dW/dt vanishes on the Hilbert space if we construct W from the $Q_{ab}(\lambda)$ defined in section 3 and arrange that W is self-adjoint on the same $\mathcal{H} = \mathcal{L}^2(R^{3n})$ as are the Q_{ab} . As one can differentiate the $Q_{ab}(\lambda)$ with respect to λ , and t , it is in principle straightforward to investigate the dependence of W and its matrix elements upon λ and t in the neighbourhood of $\lambda = 0, t = \tau, -\infty < \tau < \infty$. However the sense in which a power series in either or both of these variables approximates the original function W for times in the remote past or future must be investigated separately in each case.

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RESUMEN

Las constantes del movimiento Q , en mecánica cuántica, se definen como invariantes locales de una ecuación del movimiento cuántica. Ellas son inherentemente, objetos más generales que los invariantes considerados en la teoría de Lie-Ovsjannikov sobre la simetría de ecuaciones diferenciales. Se muestra que para una clase grande e importante de hamiltonianos de Schroedinger H_0 y $H(\lambda)$, λ un parámetro, hay una correspondencia continua uno a uno, entre las constantes del movimiento Q_{i_0} y $Q_i(\lambda)$ para todo tiempo finito. Se aísla y evita el análogo cuántico de las discontinuidades que encontró Poincaré en las primeras integrales clásicas, del problema de los n cuerpos. Entonces, se pueden definir útilmente los conceptos de "constante del movimiento aproximada" e "invariante aproximada de una ecuación de Schroedinger", y se pueden relacionar las propiedades algebraicas de sistemas perturbados con aquellas del sistema sin perturbar.