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LETTER TO THE EDITOR

Canonical transformations to action and angle variables and their representations

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Abstract. A representation on Hilbert space of canonical transformations to action and angle variables is given for a wide class of one-dimensional periodic motions. This extends the results discussed previously for the harmonic oscillator to problems not solvable in closed form. The concepts of ambiguity group and ambiguity spin continue to play a key role.

In recent papers (Moshinsky and Seligman 1978a, b, 1979; referred to hereafter as MS1, MS2 and MS3) the authors have been interested in the representation in quantum mechanics of canonical transformations leading to action and angle variables. This is part of a general programme for representations of all (nonlinear as well as linear (Moshinsky and Quesne 1971)) canonical transformations.

So far we have been able to obtain the above representations for specific problems associated with the one-degree-of-freedom Hamiltonians of the oscillator (MS1) (both attractive and repulsive), free particle (MS1) and particle in a Coulomb potential (MS3). All these problems can be solved exactly, both in classical and quantum mechanics, and our proofs (MS1–3) were based on their explicit dynamical groups or, more specifically, on their spectrum-generating algebras.

The purpose of this Letter is to show that the problem may be treated in a quite general fashion using semi-classical approximations as given in standard textbooks (Landau and Lifshitz 1959). We shall specifically consider Hamiltonians giving rise to closed orbitals only, as these are the cases where action variables can always be defined (Goldstein 1957). Also we wish to avoid singularities in this brief communication, and thus we propose a Hamiltonian of the form

$$H(q,p)=\tfrac{1}{2}p^2+V(q), \tag{1}$$

where the mass of the particle is 1, and the potential $V(q)$ is a continuous function of q bounded from below and increasing monotonically to ∞ for $|q|\to\infty$ on both sides of a single minimum. Without loss of generality we may choose this minimum at $q=0$ with $V(0)=0$. Obviously the motion is periodic, and thus the corresponding quantum-mechanical Hamiltonian (for which we take $\hbar=1$ and replace p by $-\mathrm{i}\partial/\partial q$) has only a discrete spectrum.

Before proceeding further, we wish to remark that reference MS1 will be the basis for understanding this paper, with the change—discussed in MS2 and MS3—that our solutions will be presented in configuration rather than momentum space.

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To determine the action and angle variables for the H of equation (1) we first note that the canonically conjugate variable to H is the time $t(q, p)$ defined by

$$t(q,p) = \int [2(H - V(q))]^{-1/2}\, \mathrm{d}q, \tag{2}$$

where *after* carrying out the integration H is replaced by its value on the right-hand side of (1). Clearly (Goldstein 1975) then t and H are canonically conjugate variables.

In turn the action variable can be defined by (Goldstein 1975)

$$|Q| = (2\pi)^{-1} \oint p\, \mathrm{d}q = \pi^{-1} \int_{q_-}^{q_+} [2(H - V(q))]^{1/2}\, \mathrm{d}q \equiv J(H), \tag{3}$$

where q_+, q_- are the two solutions of $V(q_\pm) = H$. The integral in (3) starts from the value 0 at $H = 0$ and increases monotonically, and thus we take it as defining the absolute value (MS1–3) of the action variable $|Q|$ rather than the action variable itself. As discussed in the previous references (MS1–3), the canonically conjugate variable to $|Q|$ is not P but $PQ/|Q|$, and in this case is given by

$$PQ/|Q| = -(\mathrm{d}H/\mathrm{d}J)t(q,p) \equiv \phi(q,p). \tag{4}$$

In (4) $\phi(q, p)$ is the angle variable which obviously satisfies the Poisson bracket relation $\{\phi, J\}_{q,p} = 1$ as, from the monotonic relation between J and H, $\mathrm{d}H/\mathrm{d}J$ is the reciprocal of $\mathrm{d}J/\mathrm{d}H$.

The periodic nature of the motion then indicates that any observable $f(q, p)$ considered as a function of J, ϕ can be expanded in a Fourier series:

$$f(q,p) = \sum_{s=-\infty}^{\infty} b_s(J) \exp(\mathrm{i}s\phi). \tag{5}$$

Therefore, in particular, both q and p are amenable to this type of expansion, and from (3) and (4) we conclude that they are functions of $|Q|$ and $\exp(\mathrm{i}PQ/|Q|)$ only. As the latter are invariant under the transformations

$$Q \to Q, \qquad P \to P + 2m\pi, \qquad m \text{ integer}; \qquad Q \to -Q, \qquad P \to -P, \tag{6}$$

the mapping between the phase spaces q, p and Q, P is non-bijective (MS1).

Thus for the transformations to action and angle variables of Hamiltonians in which $V(q)$ is defined as in (1), there exists an ambiguity group, i.e. the semi-direct product $T \wedge I$ where, as indicated in (6), T are translations by $2m\pi$ and I inversions, that connect all points Q, P in the action–angle phase space mapped on a single point in the original phase space q, p. As is well known (MS1) the irreducible representations of $T \wedge I$ are characterised by a real number λ' in the interval $0 \leqslant \lambda' < 1$, and, as these representations are two-dimensional, they require also the extra index $\sigma' = \pm 1$ for the specification of its row.

As indicated in reference MS1 for the oscillator, whose potential is of the type discussed in (1), the presence of an ambiguity group requires a double infinity of sheets in the original q, p phase space to make the mapping to the new phase space Q, P bijective. In quantum mechanics this in turn implies (MS1) that the states in the original Hilbert space may be characterised by both the eigenvalue of the position operator and the indices $\lambda'\sigma'$ associated with the irreducible representation of the ambiguity group, i.e. the ambiguity spin. Thus the representation in quantum mechanics of the canonical transformation leading to action and angle variables of the oscillator (MS1), where we take the basis in which the coordinates are diagonal (MS2), is given by the matrix elements

$$\langle q', \lambda'\sigma'|U|Q'\rangle = \sum_{n=0}^{\infty} \psi_n(q')\delta(Q'-\sigma'(n+\lambda')). \tag{7}$$

In (7) we use Dirac's (1947) primed notation for the eigenvalues of *operators* associated with the corresponding classical observables, and $\psi_n(q')$ are the eigenstates of the oscillator.

The purpose of this Letter is to prove that (7) is also the representation in quantum mechanics of canonical transformations leading to action and angle variables of an arbitrary Hamiltonian of the type (1), if $\psi_n(q')$ are now interpreted as eigenstates of this Hamiltonian enumerated by $n = 0, 1, 2, \ldots$ in increasing order of the energies.

From (5) and the discussion of the corresponding paragraph, we see that all observables will be functions of $|Q|$, $\exp(iPQ/|Q|)$, and thus we proceed to determine the latter as *operators* in the original Hilbert space amplified with the indices of ambiguity spin. We can then achieve the purpose outlined in the previous paragraph if we can prove that, in the classical limit, the operators lead to the following implicit relations defining our canonical transformation:

$$|Q| = J(H(q, p)) \tag{8a}$$

$$\exp(iPQ/|Q|) = \exp(i\phi(q, p)). \tag{8b}$$

The operators (MS1) associated with $|Q|$, $\exp(iPQ/|Q|)$, in the configuration space representation (MS2), when applied to (7) give

$$|Q'| < q', \lambda'\sigma'|U|Q'\rangle = \sum_n (n+\lambda')\psi_n(q')\delta(Q'-\sigma'(n+\lambda')) \tag{9a}$$

$$\exp[(-Q'/|Q'|)\,\partial/\partial Q'] < q', \lambda'\sigma'|U|Q'\rangle = \sum_n \psi_{n-1}(q')\delta(Q'-\sigma'(n+\lambda')), \tag{9b}$$

where use was made of the fact that $\exp(a\ \mathrm{d}/\mathrm{d}x)$ translates $f(x) \to f(x+a)$, and also that from the δ function in (7) $(Q'/|Q'|) = \sigma'$. Maintaining the same notation for the operators (Dirac 1947) as for their corresponding classical observables, we obtain then the following matrix elements for the former:

$$\langle q', \lambda'\sigma'|Q|q'', \lambda''\sigma''\rangle = \sum_n (n+\lambda')\psi_n(q')\psi_n^*(q'')\delta(\lambda'-\lambda'')\delta_{\sigma'\sigma''}, \tag{10a}$$

$$\langle q', \lambda'\sigma'|\exp(iPQ/|Q|)|q'', \lambda''\sigma''\rangle = \sum_n \psi_{n-1}(q')\psi_n^*(q'')\delta(\lambda'-\lambda'')\delta_{\sigma'\sigma''}. \tag{10b}$$

We now proceed to discuss the implication of these operators in the classical limit, reviewing briefly the analysis of Landau and Lifshitz (1959) on this point. Let us take a wavefunction $\Psi(q', t)$ that represents a state whose energy has a small dispersion around an eigenvalue $E_{\bar{n}}$ of the Hamiltonian (1), where $\bar{n}$ is some large quantum number. This wavefunction can be expanded in the form

$$\Psi(q', t) = \sum_n a_n\psi_n(q')\exp(-iE_n t), \tag{11}$$

where the a_n are appreciably different from zero only in the vicinity of $\bar{n}$, and in that region they are not very sensitive to changes in n (Landau and Lifshitz 1959).

Consider now an operator related to an arbitrary observable $f(q, p)$. The expectation value of this observable with respect to the state (11) is given by

$$\bar{f}(t) = \sum_{m,n} a_m^* a_n \langle m|f|n\rangle \exp[\mathrm{i}(E_m - E_n)t], \tag{12}$$

where

$$\langle m|f|n\rangle = \int \psi_m^*(f\psi_n)\, \mathrm{d}q'. \tag{13}$$

In view of the restrictions on the wavefunction (11) we note that, by writing $m = n - s$, we can make the following assumptions (Landau and Lifshitz 1959),

$$\langle n-s|f|n\rangle \simeq \langle \bar{n}-s|f|\bar{n}\rangle, \qquad a_{n+s} \simeq a_n, \tag{14}$$

and thus from (12) and the normalisation condition $\sum_n a_n^* a_n = 1$ we get

$$\bar{f} \simeq \sum_s \langle \bar{n}-s|f|\bar{n}\rangle \exp\{\mathrm{i}s[-(\mathrm{d}H/\mathrm{d}J)t]\}. \tag{15}$$

The exponential in (15) is obtained from the fact that

$$E_{n-s} - E_n = -s\left(\frac{E_{n-s} - E_n}{(n-s)-n}\right) = -s\left(\frac{\Delta E}{\Delta n}\right), \tag{16}$$

and, in view of the restrictions on the wavefunction (11) and the relation (Landau and Lifshitz 1959) between J and n, the term in parentheses on the right-hand side of (16) can be substituted by the $\mathrm{d}H/\mathrm{d}J$ evaluated at $J = \bar{n}$.

From the definition (4) of the angle ϕ we see that in (15) we recover the classical Fourier expansion (5), where the coefficients are

$$b_s(J) = \langle \bar{n}-s|f|\bar{n}\rangle, \qquad J = \bar{n}. \tag{17}$$

We now proceed to find the classical limits of the operators associated with $|Q|$, $\exp(\mathrm{i}PQ/|Q|)$ whose matrix elements are given by (10). As discussed in references MS1–3, the unit matrix $\|\delta(\lambda' - \lambda'')\delta_{\sigma'\sigma''}\|$ is still retained in the classical limit, and so we need only consider the matrix elements of the operators associated with $|Q|$, $\exp(\mathrm{i}PQ/|Q|)$ modulo this unit matrix. From (10) and (13) we obtain

$$\langle \bar{n}-s\||Q|\|\bar{n}\rangle = \delta_{s0}\bar{n}, \tag{18a}$$

$$\langle \bar{n}-s|\exp(\mathrm{i}PQ/|Q|)|\bar{n}\rangle = \delta_{s1}, \tag{18b}$$

where we have disregarded λ' in the range $0 \leq \lambda' < 1$ as compared with $\bar{n}$. From (15), (17) and (18) we then recover the defining equations (8) of the classical canonical transformations.

We have thus proved that (7) is the representation of the canonical transformation leading to action and angle variables of a general Hamiltonian of the type (1). The concepts of ambiguity group and ambiguity spin continue to be essential in the derivation of the representation.

Furthermore we can now also represent the canonical transformation connecting two Hamiltonians of type (1) by combining the representation of the canonical transformation going to the action and angle variable of the first Hamiltonian with the inverse of the corresponding one for the second.

The arguments outlined above suggest the extension to more general Hamiltonians, where an adequate generalisation of the concept of action variable and a WKB analysis of the problems will be required. Work in this direction is under way in collaboration with J Deenen.

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