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Representation of quantum mechanical wavefunctions by transformation generators: III. Canonical transformations in an extended phase space

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Abstract. It is shown how quantum mechanical wavefunctions can be obtained from a sequence of simple canonical transformations, which map the given system onto a simple reference system. The resulting wavefunctions are at least uniformly valid up to order \hbar . Under some more restrictive conditions for the individual transformation steps we even find the exact wavefunctions. The essential point of this paper is to enlarge the conventional coordinate–momentum phase space by taking time and energy as an additional conjugate pair. In this extended phase space we exploit the possibility of using transformations which intermix energy and time with position coordinates and momenta. Compared with transformations in the conventional position–momentum phase space, we gain the advantage that scattering states and bound states can be treated in a unified way. Therefore this method is appropriate for systems with mixed spectra. In addition it allows for more flexibility in choosing the individual transformation steps. The practicability of the method is demonstrated by several examples.

1. Introduction

In two previous papers (Jung and Krüger 1982, 1983, denoted by I and II in the following) a method has been developed which provides, for a system with one degree of freedom, the quantum mechanical wavefunction in terms of the generators of an appropriate sequence of classical canonical transformations. We have used transformations in the position–momentum phase space, which map a given Hamiltonian (denoted by H_1 from now on) onto a simple reference Hamiltonian, preferably the new position coordinate. Then, in the new coordinates the description of the motion of the system is trivial, both classically and quantum mechanically. In the new coordinates the classical trajectories in phase space are straight lines. If the original system has only scattering states and therefore only unbound trajectories in the classical phase space, then these clearly can be mapped onto straight lines canonically. In § 4.1 in I we have treated the linear potential as such a case.

However, if the original system with one degree of freedom admits only bound states and therefore yields bound trajectories only in the classical phase space, then the trajectories in the original system and in the reference system, where the Hamiltonian is a cartesian coordinate, are no longer homeomorphic. A sequence of transformations which nevertheless maps bound state trajectories onto an unbound coordinate in some restricted range must therefore change the topology. This is why we used complex valued extensions of canonical transformations in I. (For the complexification

of canonical transformations see Kramer *et al* (1975).) In §§ 4.2 and 4.3 in I the harmonic oscillator was treated in this way. We obtained the exact oscillator wavefunctions with the help of complex transformation generators, which map the oscillator Hamiltonian onto a new coordinate.

Since we now wish to obtain the solutions of the Schrödinger equation with one degree of freedom for both scattering and bound states, i.e. for all values of the energy parameter, in a unified way, we are forced to treat the energy and hence the time on the same level as positions and momenta. Otherwise there is no response from position and momentum to energy and time, which restores a corresponding change in the geometry of the trajectories, if we change from bound states to scattering states. In this way we are led to extend the conventional position–momentum phase space by adding time and energy as a further conjugate pair and treating the original one degree of freedom system as a dynamical constraint in this four-dimensional position–time–momentum–energy phase space. Such a phase space extension, or embedding, is not at all new (see ch VI, § 10 in Lanczos (1970) and § E.V. in Sygne (1960)). It dates back at least to J L Lagrange and in relativistic dynamics it has become an absolute necessity.

In the present paper the Schrödinger equation with one degree of freedom is solved for particular systems by a sequence of canonical transformations, which intermix all four variables, the coordinates of the extended phase space. Thereby a system with one degree of freedom is treated in the extended phase space like a system with two degrees of freedom in the conventional position–momentum phase space. For canonical transformations in the extended phase space already the generator of the first transformation step depends on the energy explicitly and therefore there is no difficulty in changing the topological properties of the transformation in an energy-dependent way, in order to switch from bound to unbound trajectories or *vice versa*. These ideas are presented in full detail in the following four sections of this paper. In § 2 we explain our notation, and give the basic formulae for the quantum mechanical transformation kernels and their composition. In § 3 we derive sufficient conditions that have to be imposed on the various intermediate transformations in order that a sequence of them yields a uniform semiclassical or even exact solution of the corresponding Schrödinger equation. Section 4 contains some examples and in § 5 we draw further conclusions and give some final remarks.

2. Composition of canonical transformations in quantum mechanics

We study the composition of $N - 1$ canonical transformations, thus defining a sequence of N coordinate systems in the four-dimensional extended phase space introduced in § 1. We treat this extended phase space of a system with one degree of freedom like the conventional four-dimensional position–momentum phase space of a system with two degrees of freedom, and use the notation developed in I, II with some minor extensions, which are explained in the following.

q_k^l and p_k^l are the position and momentum coordinates in coordinate system k , $l = 1, 2$ denotes the two components of q and p or the two degrees of freedom; q_k^1 is position, q_k^2 energy, p_k^1 momentum and p_k^2 time. q_k or p_k without a superscript means the two-component vectors $q_k = (q_k^1, q_k^2)$ or $p_k = (p_k^1, p_k^2)$. \hat{q}_k^l and \hat{p}_k^l are the corresponding quantum mechanical operators. $|q_k(x)\rangle = |q_k^1(x^1), q_k^2(x^2)\rangle$ and $|p_k(y)\rangle = |p_k^1(y^1), p_k^2(y^2)\rangle$ are the eigenstates of the operators \hat{q}_k and \hat{p}_k with eigenvalues x and

y, i.e.

$$\hat{q}_k^l |q_k(x)\rangle = x^l |q_k(x)\rangle, \quad \hat{p}_k^l |p_k(y)\rangle = y^l |p_k(y)\rangle. \tag{1}$$

Coordinate system 1 consists of the standard cartesian coordinates. The problem we wish to solve is given in coordinate system 1 by a Hamiltonian function $H_1(q, p, t)$ classically or a Hamilton operator $\hat{H}_1(x, (\hbar/i) d/dx, t)$ quantum mechanically. In the extended phase space this problem is classically defined by the dynamical constraint $\Omega_1(q_1^1, p_1^1, q_1^2, p_1^2) = 0$, where

$$\Omega_1(q_1^1, p_1^1, q_1^2, p_1^2) = H_1(q_1^1, p_1^1, p_1^2) - q_1^2.$$

The quantum version consists in finding solutions ψ_1 of the Schrödinger equation

$$\hat{\Omega}_1 \psi_1 = 0. \tag{2}$$

We obtain H and Ω in coordinate system k by inserting q_1 and p_1 as functions of q_k and p_k into H_1 and Ω_1 , i.e.

$$\Omega_k(q_k, p_k) = \Omega_1(q_1(q_k, p_k), p_1(q_k, p_k)).$$

Our aim is, in complete analogy to the classical transformation theory of Jacobi, to map onto a coordinate system N in which Ω_N has such a simple form that the solution of $\hat{\Omega}_N \psi_N = 0$ is obvious (see also Falk 1952). Then ψ_1 is given by the transformation which maps ψ_N back to ψ_1 , i.e.

$$\psi_1(x) = \int \chi^{1 \leftarrow N}(x, y) \psi_N(y) dy$$

where $\chi^{1 \leftarrow N}$ is the transformation kernel of the total transformation combining the whole sequence of intermediate steps. Therefore, the central point of this paper is the construction of $\chi^{1 \leftarrow N}$ out of transformation generators.

For each transformation step the corresponding transformation kernel is the scalar product of the eigenstates of the old \hat{q}_k or \hat{p}_k with the eigenstates of the new \hat{q}_{k+1} or \hat{p}_{k+1} . It is not possible to give these matrix elements for all canonical transformations in terms of known functions. However, it has been shown by Miller (1974) how all these matrix elements can be obtained semiclassically at least in closed form; they are a function of the classical generator of the transformation only (see equations (2.50) and (2.51) in Miller 1974). In the following we shall define all transformations by generators of type 2 or 3 (for the representation of canonical transformations by generators see § 48 in Arnold (1978)). F_2^k , the generator of type 2 which defines the transformation from coordinate system k to coordinate system $k + 1$, is a function of the old position and new momentum, i.e. $F_2^k(q_k, p_{k+1})$. F_3^l is a function of p_j and q_{j+1} . In this notation Miller's equation for the transformation kernel is

$$\varphi^k(x, y) = \langle q_k(x) | p_{k+1}(y) \rangle = (2\pi\hbar)^{-1} [\det(\partial^2 F_2^k(x, y) / \partial x \partial y)]^{1/2} \exp[(i/\hbar) F_2^k(x, y)] \tag{3}$$

with a similar expression involving F_3 for $\langle p_j(y) | q_{j+1}(x) \rangle$. φ^k is the kernel of the integral transform which maps the wavefunction ψ_{k+1} of \hat{H}_{k+1} onto the wavefunction ψ_k of \hat{H}_k ,

$$\psi_k(x) = \int \varphi^k(x, y) \psi_{k+1}(y) dy.$$

If the one-step transformation between coordinate system k and $k + 1$ would map the given problem onto the reference system for which $\hat{H}_{k+1} = \hat{q}_{k+1}$, then $\langle q_k | q_{k+1} \rangle$ would already be the wavefunction of the original problem.

In general (3) is valid only semiclassically and, even worse, the determinant gives rise to caustic singularities and the resulting wavefunction would not be suited for many applications. Therefore a one-step transformation gives a semiclassical approximation which is too crude to be useful in most cases. In I we have shown that if the generator F is linear in the new variable, then (3) is quantum mechanically exact. Accordingly, we divide the transformation from a given system to a simple reference problem into a sequence of simple steps with this linearity property, and thereby obtain wavefunctions which are exact, or at least valid as uniform semiclassical approximations, i.e. without caustic singularities. In § 3 we show that the same holds for transformations in the extended four-dimensional phase space.

Without loss of generality we may always assume that the total number of transformation steps in a sequence is even and that the various intermediate steps are defined by generators of type 2 and 3 alternately. This ensures that the new variables in F^k are the same as the old variables in F^{k+1} . The transformation kernel after a composition of two steps is then

$$\begin{aligned} \chi^{1 \leftarrow 3}(x, z) &= \int dy \varphi^1(x, y) \varphi^2(y, z) \\ &= \iint dy^1 dy^2 \varphi^1(x^1, x^2, y^1, y^2) \varphi^2(y^1, y^2, z^1, z^2) \end{aligned} \quad (4)$$

where φ^k has been defined by (3).

For an arbitrary number of steps we thus obtain

$$\chi^{1 \leftarrow n+1}(x, z) = \int dy \chi^{1 \leftarrow n}(x, y) \varphi^n(y, z). \quad (5)$$

In order to avoid boundary contributions from intermediate partial integrations, we choose the integration domains in such a way that the integrand vanishes sufficiently fast at the boundaries of all integration sets or that the integration domains are cycles in complex valued extensions of the integration regions. If the integrations are extended to infinity, then we require that the integrand vanishes exponentially along any direction in the integration domain. The further specification of the integration paths clearly depends on the boundary conditions imposed on ψ_1 . In the present paper we are only interested in constructing solutions to the differential equation (2) and do not care about particular boundary conditions.

3. Exactness conditions

The exact transformation kernels are characterised by the property of being solutions of certain differential equations. A compilation of these equations for transformations given by generators of the various types has been given by Eckelt (1979, equations (2.12)–(2.15)). Even though these equations have been derived for the case of one degree of freedom, it is obvious that they hold component-wise also for several degrees of freedom. One needs only to attach component indices to the q , Q , p and P variables which occur in Eckelt's equations. For the individual transformation steps we need

equations for generators of type 2 and 3. The composition of an even number of alternating F_2 and F_3 transformations then results in a kernel, which maps from an old position eigenstate to a new position eigenstate. This kernel must fulfil the same equations as a kernel given by a one-step transformation defined by a generator of type 1, which is a function of the old and new position variables. Therefore we need the exactness conditions for the F_1 case too. All these conditions are now displayed for later reference. The notation $q_k^i(q_l, p_l)$ and $p_k^i(q_l, p_l)$ indicates that the q^i and p^i coordinates in coordinate system k are expressed as functions of the coordinates in coordinate system l .

Type 1. $\varphi(x, y) = \langle q_k(x) | q_l(y) \rangle$ is exact if it satisfies

$$(\hbar/i)(\partial/\partial y^j)\varphi(x, y) = -p_l^j(\hat{q}_k, \hat{p}_k)\varphi(x, y), \tag{6a}$$

$$y^j\varphi(x, y) = q_l^j(\hat{q}_k, \hat{p}_k)\varphi(x, y), \tag{6b}$$

where $\hat{q}_k^i = x^i, \hat{p}_k^i = (\hbar/i) \partial/\partial x^i$.

Type 2. $\varphi(x, y) = \langle q_k(x) | p_l(y) \rangle$ is exact if it satisfies

$$(\hbar/i)(\partial/\partial y^j)\varphi(x, y) = q_l^j(\hat{q}_k, \hat{p}_k)\varphi(x, y), \tag{7a}$$

$$y^j\varphi(x, y) = p_l^j(\hat{q}_k, \hat{p}_k)\varphi(x, y), \tag{7b}$$

where \hat{q}_k, \hat{p}_k is the same as for type 1.

Type 3. $\varphi(x, y) = \langle p_k(x) | q_l(y) \rangle$ is exact if it satisfies

$$(\hbar/i)(\partial/\partial y^j)\varphi(x, y) = -p_l^j(\hat{q}_k, \hat{p}_k)\varphi(x, y), \tag{8a}$$

$$y^j\varphi(x, y) = q_l^j(\hat{q}_k, \hat{p}_k)\varphi(x, y), \tag{8b}$$

where $\hat{q}_k^i = i\hbar \partial/\partial x^i, \hat{p}_k^i = x^i$.

Now we present a condition which guarantees that (7) are satisfied by the kernel defined in (3).

Proposition 1. Let the transformation be defined by the generator

$$F_2^k(q_k, p_{k+1}) = p_{k+1}^1 f_1(q_k) + p_{k+1}^2 f_2(q_k) + g(q_k) \tag{9}$$

where f_1, f_2, g are any differentiable functions of q_k . For the transformation to be non-singular we require that the determinant of the mixed second derivative of F is non-zero, i.e.

$$\det \frac{\partial^2 F}{\partial q_k \partial p_{k+1}} = \frac{\partial f_1}{\partial q_k^1} \frac{\partial f_2}{\partial q_k^2} - \frac{\partial f_1}{\partial q_k^2} \frac{\partial f_2}{\partial q_k^1} \neq 0. \tag{10}$$

If (9) and (10) are fulfilled, then the transformation kernel given by (3) fulfils (7a), (7b).

Proof.

$$q_{k+1}^i = \partial F / \partial p_{k+1}^i = f_i(q_k), \tag{11}$$

$$p_k^i = \frac{\partial F}{\partial q_k^i} = p_{k+1}^1 \frac{\partial f_1}{\partial q_k^i} + p_{k+1}^2 \frac{\partial f_2}{\partial q_k^i} + \frac{\partial g}{\partial q_k^i}. \tag{12}$$

We introduce $A_{ij} = \partial f_j / \partial q_k^i$. Because of (10), $\det A \neq 0$ hence

$$A^{-1} = B = \frac{1}{\det A} \begin{pmatrix} A_{22} & -A_{21} \\ -A_{12} & A_{11} \end{pmatrix}.$$

We further note that

$$\sum_j \frac{\partial}{\partial q_k^j} B_{ij}(q_k) = - \sum_j B_{ij}(q_k) \frac{1}{\det A(q_k)} \frac{\partial}{\partial q_k^i} \det A(q_k) \tag{13}$$

which follows on calculating the derivatives of the matrix elements of B . With the help of B we may resolve (12) for p_{k+1}^i ,

$$p_{k+1}^i = \sum_j (p_k^j - \partial g / \partial q_k^j) B_{ij}. \tag{14}$$

In general B is a function of q_k , therefore it is necessary to choose an appropriate order of the factors in (14) if an operator version of (14) is considered in which q_k is the multiplication operator and p_k is a derivative operator. Because p_k appears linearly in (14) the choice of any symmetric order is sufficient, e.g.

$$\hat{p}_{k+1}^i = \frac{1}{2} \sum_j (\hat{p}_k^j - g(\hat{q}_k) / \partial \hat{q}_k^j) B_{ij}(\hat{q}_k) + \frac{1}{2} \sum_j B_{ij}(\hat{q}_k) (\hat{p}_k^j - \partial g(\hat{q}_k) / \partial \hat{q}_k^j). \tag{15}$$

\hat{p}_{k+1} applied to any function φ of q_k gives

$$\begin{aligned} \hat{p}_{k+1}^i \varphi(q_k) &= \sum_j B_{ij}(q_k) \frac{\hbar}{i} \frac{\partial}{\partial q_k^j} \varphi(q_k) \\ &+ \frac{1}{2} \sum_j \frac{\hbar}{i} \left(\frac{\partial}{\partial q_k^j} B_{ij}(q_k) \right) \varphi(q_k) - \sum_j B_{ij}(q_k) \left(\frac{\partial}{\partial q_k^j} g(q_k) \right) \varphi(q_k). \end{aligned} \tag{16}$$

According to (3), φ^k is

$$\begin{aligned} \varphi^k(x, y) &= (2\pi\hbar)^{-1} [\det A(x)]^{1/2} \exp \left[(i/\hbar) \left(\sum_j y^j f_j(x) + g(x) \right) \right], \tag{17} \\ (\hbar/i)(\partial/\partial y^l) \varphi^k(x, y) &= f_l(x) \varphi^k(x, y). \end{aligned}$$

Comparison with (11) shows that (7a) is fulfilled:

$$\frac{\hbar}{i} \frac{\partial}{\partial x^l} \varphi^k(x, y) = \left[\frac{\hbar}{2i} \frac{1}{\det A(x)} \left(\frac{\partial}{\partial x^l} \det A(x) \right) + \sum_j y^j A_{lj} + \frac{\partial g(x)}{\partial x^l} \right] \varphi(x, y).$$

Multiplication by $B_{n,l}$, summation over l , using (13) and the fact that $\sum_l B_{nl} A_{lj} = \delta_{n,j}$ then leads to

$$y^n \varphi(x, y) = \sum_l B_{nl} \frac{\hbar}{i} \frac{\partial}{\partial x^l} \varphi(x, y) - \sum_l B_{nl} \left(\frac{\partial g(x)}{\partial x^l} \right) \varphi(x, y) + \sum_l \frac{\hbar}{2i} \left(\frac{\partial}{\partial x^l} B_{nl}(x) \right) \varphi(x, y).$$

Comparison with (16) shows that (7b) is fulfilled.

Remarks.

(1) For generators of any other type an analogous proposition holds, i.e. a sufficient condition for exactness of (3) is that the generator F is a linear function of the new coordinate occurring in F . This linearity leads to the following two essential properties.

(a) The determinant depends on the old variable only. This avoids caustic singularities.

(b) p_{k+1} in (14) is a linear function of p_k . This allows a simple ordering prescription (15) or analogous expressions for generators of the other types.

Analogous conclusions hold if F is a linear function of the old coordinate occurring in F .

(2) The transformation kernel φ remains exact if a function of the new variable only is added to the generator. But it is not necessary to take into account this generalisation, because it is always possible to shift any function of the new variable only into the generator of the next step of the composite transformation. We repeat this statement as:

Proposition 2. Let $h(p_2)$ be a differentiable function of p_2 and F_2^1 and F_3^2 be two transformation generators, which are linear in the new variables and give rise to non-singular transformations. Then, the two sequences of transformations from coordinate system 1 to coordinate system 3 given by the generators $F_2^1(q_1, p_2)$ and $F_3^2(p_2, q_3)$ in one case and $\tilde{F}_2^1(q_1, p_2) = F_2^1(q_1, p_2) + h(p_2)$, $\tilde{F}_3^2(p_2, q_3) = F_3^2(p_2, q_3) - h(p_2)$ in the other case lead to the same expressions of q_3, p_3 in terms of q_1, p_1 .

This proposition can be proven by straightforward calculation of q_3, p_3 in both cases.

If several steps of the form (9) or an analogous form for generators of type 3 are composed, then the integral representation (4), (5) of the total transformation kernel is not exact in general. Inserting one transformation step into the previous one causes ordering problems in the operator case which are not treated exactly by the composition rules (4) and (5), if the generators are of the form (9). In the total transformation kernel this may cause errors of order \hbar^2 or higher. To ensure exactness of the composed total kernel we may impose stronger requirements on the transformation generators and formulate:

Proposition 3. If in a sequence of canonical transformations all generators have a constant determinant of the second mixed derivatives, then (3)–(5) provide the exact quantum mechanical transformation kernel χ . χ remains exact if at most one generator is of the more general form (9).

This is in complete analogy to proposition 3 in I and may be proven in the same way. We do not give a proof here, because the conditions in proposition 3 are of little practical value. In all the examples investigated in § 4 we need several transformation steps, whose determinants are not constant. In addition, these conditions are only sufficient but not necessary. In § 4 we shall see that there exist non-trivial examples for which these sufficient conditions are not fulfilled, but where the resulting transformation kernels and wavefunctions are nevertheless exact. Unfortunately, so far we have not been able to find both necessary and sufficient conditions for the multistep transformations to provide the exact total transformation kernel.

4. Examples

This section contains a few examples for the transformation technique developed in the previous sections. For simplicity we take examples which can be solved with small effort by conventional methods. Therefore it is easy to compare our results with the standard solutions.

4.1. *The two-dimensional oscillator*

Before we give examples for transformations in the extended phase space, we start with the two-dimensional isotropic harmonic oscillator for the following two reasons.

(1) We treat the extended phase space for a system with one degree of freedom like the normal position-momentum phase space of a system with two degrees of freedom. Therefore, it is useful to gain some experience in handling transformations in this four-dimensional phase space.

(2) The following example uses the two-dimensional oscillator as reference system. So, the transformations given in this example are steps which can be added to the transformations of the next example in order to map the next example onto the position variable in the final coordinate system. In this sense the present example is an intermediate step for the next example.

Let the Hamiltonian function of the two-dimensional oscillator be given by

$$H_1(q_1, p_1) = (p_1^2)/2m + (p_1^2)^2/2m + \frac{1}{2}m\omega^2(q_1^2) + \frac{1}{2}m\omega^2(q_1^2)^2. \tag{18}$$

This Hamiltonian separates in coordinate system 1 and it could be mapped onto $H_3(q_3, p_3) = q_3^4 + p_3^2$ by applying the transformations used in § 4.2 in I. This, however, would not provide any new insight into transformations which intermix the two degrees of freedom and in addition it would not represent the resulting wavefunction in the form which is most useful for the next example. Instead, we shall map H_1 onto $H_5(q_5, p_5) = q_5^4$ in such a way that the resulting wavefunction is given in two-dimensional polar coordinates. Therefore, as the first transformation step we introduce polar coordinates according to

$$F_2^1(q_1, p_2) = p_2^1[(q_1^1)^2 + (q_1^2)^2]^{1/2} + p_2^2 \tan^{-1}(q_1^2/q_1^1), \tag{19}$$

$$\det \frac{\partial^2 F}{\partial q_1 \partial p_2} = [(q_1^1)^2 + (q_1^2)^2]^{-1/2} = (q_1^2)^{-1}.$$

For a more convenient calculation of the integrals occurring in the integral representation of the composite kernel, we insert in the next step the identity transformation

$$F_3^2(p_2, q_3) = -p_2^1 q_3^1 - p_2^2 q_3^2, \quad \det \partial^2 F / \partial p_2 \partial q_3 = 1, \tag{20}$$

$$H_3(q_3, p_3) = (p_3^1)^2/2m + (p_3^2)^2/2m + q_3^4 + \frac{1}{2}m\omega^2(q_3^1)^2.$$

To map H_3 onto H_5 we use essentially the same two transformations as in § 4.3 in I, namely

$$F_2^3(q_3, p_4) = im\omega(q_3^1)^2 p_4^1 + \frac{1}{2}im\omega(q_3^1)^2 - ip_4^2 \ln(q_3^1/x_0) + q_3^2 p_4^2,$$

$$\det \partial^2 F / \partial q_3 \partial p_4 = 2im\omega q_3^1,$$

$$F_3^4(p_4, q_5) = (1/2i)(p_4^2 - q_5^1/\omega) \ln(p_4^1) + (1/2i)(p_4^2 + q_5^1/\omega) \ln(p_4^1 + 1) - p_4^2 q_5^2,$$

$$\det \partial^2 F / \partial p_4 \partial q_5 = [2i\omega p_4^1(p_4^1 + 1)]^{-1}, \quad H_5(q_5, p_5) = q_5^4. \tag{21}$$

Now the Hamilton function is in the simplest form and it is obvious that the solution of the Schrödinger equation is given by the δ -distribution $\delta(q_5^1 - E)$, because of

$$\hat{H}_5(q_5, p_5) \delta(q_5^1 - E) = \hat{q}_5^4 \delta(q_5^1 - E) = q_5^4 \delta(q_5^1 - E) = E \delta(q_5^1 - E).$$

This gives the solution of the Schrödinger equation for any value of the energy E . These δ -distributions are not yet sufficiently definite solutions, because they do not depend on the variable of the second degree of freedom. We have started from an

integrable system with two degrees of freedom, and therefore a definite solution may be characterised as an eigenfunction of two commuting operators. Equation (21) shows that any function of q_5^2 and p_5^2 commutes with H_5 and accordingly any function of q_5^2 and p_5^2 can be chosen as second conserved quantity. An interesting choice is the angular momentum $L_5 = p_5^2$. So, a definite wavefunction in coordinate system 5 is given by

$$\psi_5(q_5^1, q_5^2 | E, F) = \exp[(i/\hbar)Fq_5^2]\delta(q_5^1 - E) \tag{22}$$

which fulfils

$$\begin{aligned} \hat{H}_5\psi_5 &= q_5^1\psi_5 = E\psi_5, \\ \hat{L}_5\psi_5 &= \hat{p}_5^2\psi_5 = (\hbar/i)(\partial/\partial q_5^2)\psi_5 = F\psi_5. \end{aligned}$$

The transformation from ψ_5 back to ψ_1 in coordinate system 1 is arranged by the kernel $\chi^{1\leftarrow 5}$, which will be built now by application of (3)–(5). Because we are not interested in normalisation, we put all unimportant constant factors into an unspecified normalisation constant \mathcal{N} .

$$\begin{aligned} \chi^{1\leftarrow 5}(q_1, q_5) &= \mathcal{N} \int \int \int \int \int \int \int d\alpha d\beta d\gamma d\delta d\varepsilon d\zeta \gamma^{1/2} \\ &\times [(q_1^1)^2 + (q_1^2)^2]^{-1/4} [\varepsilon(\varepsilon + 1)]^{-1/2} \exp \left[\frac{i}{\hbar} \alpha [(q_1^1)^2 + (q_1^2)^2]^{1/2} \right. \\ &+ \frac{i}{\hbar} \beta \tan^{-1} \left(\frac{q_1^2}{q_1^1} \right) - \frac{i}{\hbar} \alpha \gamma - \frac{i}{\hbar} \beta \delta - \frac{m\omega}{\hbar} \gamma^2 \varepsilon - \frac{m\omega}{2\hbar} \gamma^2 + \frac{\zeta}{\hbar} \ln \left(\frac{\gamma}{x_0} \right) \\ &\left. + \frac{i}{\hbar} \delta \zeta + \frac{1}{2\hbar} \left(\zeta - \frac{q_5^1}{\omega} \right) \ln \varepsilon + \frac{1}{2\hbar} \left(\zeta + \frac{q_5^1}{\omega} \right) \ln(\varepsilon + 1) - \frac{i}{\hbar} \zeta q_5^2 \right]. \tag{23} \end{aligned}$$

The first two transformations are real and the transformation of p_4^2 in the third transformation step is real. Therefore $\alpha, \beta, \gamma, \delta, \zeta$ (the eigenvalues of $p_2^1, p_2^2, q_3^1, q_3^2, p_4^2$) are integrated over the real axis. The transformation of p_4^1 in the third transformation step is complex. Therefore ε (the eigenvalue of p_4^1) is integrated along a path in the complex plane. We use the same path as in §§ 4.2 and 4.3 in I and § 4.1 in II: it starts from infinity along the positive real axis, encircles the origin once along the boundary of a circle of radius smaller than 1 and then tends back to infinity along the positive real axis of the next sheet of the Riemann surface belonging to the branch point at $\varepsilon = 0$. Note that the integrand goes to zero exponentially as the path goes to infinity and that the path does not hit a singularity of the integrand.

The $\alpha, \beta, \gamma, \delta$ integrations in (23) can be done easily. Using the abbreviations $r = [(q_1^1)^2 + (q_1^2)^2]^{1/2}$ and $\varphi = \tan^{-1}(q_1^2/q_1^1)$, we find

$$\begin{aligned} \chi^{1\leftarrow 5}(q_1, q_5) &= \mathcal{N} \int \int d\varepsilon d\zeta r^{\zeta/\hbar} \varepsilon^{(-1/2 + \zeta/2\hbar - q_5^1/2\hbar\omega)} \\ &\times (\varepsilon + 1)^{(-1/2 + \zeta/2\hbar + q_5^1/2\hbar\omega)} \exp \left(-\frac{m\omega}{2\hbar} r^2(1 + 2\varepsilon) + \frac{i}{\hbar} \varphi \zeta - \frac{i}{\hbar} \zeta q_5^2 \right). \tag{24} \end{aligned}$$

Thus ψ_1 becomes

$$\psi_1(q_1^1, q_1^2, E, F) = \int \int dq_5^1 dq_5^2 \chi^{1\leftarrow 5}(q_1, q_5) \psi_5(q_5^1, q_5^2 | E, F)$$

and insertion of (22) and (24) gives

$$\psi_1(r, \varphi|E, F) = \mathcal{N}r^{F/\hbar} \exp[(i/\hbar)F\varphi] \int d\varepsilon \varepsilon^{(-1/2+F/2\hbar-E/2\hbar\omega)} \times (\varepsilon + 1)^{(-1/2+F/2\hbar+E/2\hbar\omega)} \exp[-(m\omega/2\hbar)r^2(1 + 2\varepsilon)]. \tag{25}$$

As direct calculation shows, the wavefunction ψ_1 is an exact solution of the equations

$$\hat{H}_1\psi_1 = E\psi_1, \quad \hat{L}_1\psi_1 = F\psi_1.$$

The correct quantisation of the values of F and E can be obtained from (25) by imposing uniqueness requirements. ψ_1 has no branch point at $r = 0$ if F/\hbar is integer, i.e. if the conventional angular momentum quantisation is satisfied. Therefore we put $F/\hbar = l \in \mathbb{Z}$.

For $l \geq 0$ we obtain the solution which is regular at the origin and for $l < 0$ we obtain a solution which is singular at the origin. In order to obtain a second linearly independent solution for each l we can replace the generators F_3^2 and F_3^4 by

$$\begin{aligned} \tilde{F}_3^3(q_3, p_4) &= im\omega(q_3^1)^2 p_4^1 + \frac{1}{2}im\omega(q_3^1)^2 + ip_4^2 \ln(q_3^1/x_0) + q_3^2 p_4^2, \\ \tilde{F}_3^4(p_4, q_5) &= (2i)^{-1}(-p_4^2 - q_5^1/\omega) \ln(p_4^1) + (2i)^{-1}(-p_4^2 + q_5^1/\omega) \ln(p_4^1 + 1) - p_4^2 q_5^2. \end{aligned}$$

This change of sign does not have any influence on the mapping of H_3 onto $H_5 = q_5^1$. Performing with the new generators the same steps as before leads to

$$\tilde{\psi}_1(r, \varphi|E, F) = \mathcal{N}r^{-F/\hbar} \exp[(i/\hbar)F\varphi] \int d\varepsilon \varepsilon^{(-1/2-F/2\hbar-E/2\hbar\omega)} \times (\varepsilon + 1)^{(-1/2-F/2\hbar+E/2\hbar\omega)} \exp[-m\omega r^2(1 + 2\varepsilon)/2\hbar]. \tag{25'}$$

Also this function is an exact solution of the Schrödinger equation and it is an eigenfunction of the angular momentum with eigenvalue F . Equation (25') gives a solution which is singular at the origin for $l > 0$ and the solution which is regular at the origin for $l \leq 0$.

Further, the integrand in (25) or (25') has no branch point at $\varepsilon = 0$, if $A = -\frac{1}{2} + l/2 - E/2\hbar\omega \in \mathbb{Z}$ in the case of (25) or if $A = -\frac{1}{2} - l/2 - E/2\hbar\omega \in \mathbb{Z}$ in the case of (25'). If A is a positive integer or zero, then the ε integral vanishes. If A is a negative integer, then the integrand has a pole at $\varepsilon = 0$ and the integration path can be deformed to the boundary of a circle around the origin, yielding a single-valued ψ_1 .

If we are only interested in regular functions we can combine the conditions for (25) and (25') and obtain the following result. There is a single-valued, regular, wavefunction for all values of F and E such that $F/\hbar = l \in \mathbb{Z}$ and $A = -\frac{1}{2} + |l|/2 - E/2\hbar\omega \in \mathbb{Z}$, and $A < 0$.

This condition is equivalent to

$$E = \hbar\omega(2n + |l| + 1) \quad \text{with } n = 0, 1, 2, \dots$$

One notes that this condition gives the correct energy eigenvalues of the two-dimensional oscillator.

4.2.

The next example is the Morse system defined by

$$\Omega_1 = (p)^2/2m + D e^{-2q/x_0} - 2D e^{-q/x_0} - E. \tag{26}$$

We put $q = q_1^1, p = p_1^1, E = q_1^2, t = p_1^2$. The first transformation step removes the exp functions by

$$\begin{aligned} F_2^1(q_1, p_2) &= x_0 p_2^1 \exp(-q_1^1/2x_0) + x_0 p_2^2 (-8mq_1^2)^{1/2}, \\ \det \partial^2 F / \partial q_1 \partial p_2 &= -mx_0 (-2mq_1^2)^{-1/2} \exp(-q_1^1/2x_0), \\ \Omega_2 &= \frac{(p_2^1 q_2^1)^2}{8mx_0^2} + \frac{D(q_2^1)^4}{x_0^4} - 2D \frac{(q_2^1)^2}{x_0^2} + \frac{(q_2^2)^2}{8mx_0^2}. \end{aligned} \quad (27)$$

By the next two transformation steps we replace q_2^2 by p_4^2 and keep the variables of the first degree of freedom the same:

$$\begin{aligned} F_3^2(p_2, q_3) &= -p_2^1 q_3^1 + p_2^2 q_3^2 + (p_2^2)^2/2, \\ F_2^3(q_3, p_4) &= q_3^1 p_4^1 + q_3^2 p_4^2 + (q_3^2)^2/2. \end{aligned}$$

Both these transformations have determinant 1:

$$\Omega_4 = \frac{(q_4^1)^2}{4x_0^2} \left(\frac{(p_4^1)^2}{2m} + 4D \frac{(q_4^1)^2}{x_0^2} - 8D + \frac{(p_4^2)^2}{2m(q_4^1)^2} \right).$$

As a last step we apply the transformation from polar coordinates to cartesian coordinates. This is the inverse of the first transformation step in § 4.1:

$$\begin{aligned} F_3^4(p_4, q_5) &= -p_4^1 [(q_5^1)^2 + (q_5^2)^2]^{1/2} - p_4^2 \tan^{-1}(q_5^2/q_5^1), \\ \det \partial^2 F / \partial p_4 \partial q_5 &= [(q_5^1)^2 + (q_5^2)^2]^{-1/2}, \\ \Omega_5 &= \frac{(q_5^1)^2 + (q_5^2)^2}{4x_0^2} \left[\frac{(p_5^1)^2}{2m} + \frac{(p_5^2)^2}{2m} + 4D \frac{(q_5^1)^2}{x_0^2} + 4D \frac{(q_5^2)^2}{x_0^2} - 8D \right]. \end{aligned} \quad (28)$$

In analogy to the previous example we shall use again the abbreviations $r = [(q_5^1)^2 + (q_5^2)^2]^{1/2}$ and $\varphi = \tan^{-1}(q_5^2/q_5^1)$. According to (4) and (5) the total transformation kernel is given by

$$\chi^{1 \leftarrow 5}(q, E, r, \varphi) = \mathcal{N}(E) \delta(x_0 e^{-q/2x_0} - r) \exp[-(i/\hbar)\varphi(-8mE)^{1/2}x_0]. \quad (29)$$

In this expression the original variables q and E have been used and all uninteresting factors have been combined into an energy-dependent normalisation factor $\mathcal{N}(E)$.

The square bracket in (28) is just the Ω function of the two-dimensional oscillator (compare (18)), if the following replacements are made:

$$4D/x_0^2 \rightarrow \omega^2 m/2 \quad \text{and} \quad 8D \rightarrow E. \quad (30)$$

Accordingly, the wavefunctions which are mapped onto zero by the operator version of the square bracket are given in (25). In order to be able to select in a unique way which wavefunctions are mapped onto zero by $\hat{\Omega}_5$, it is necessary to keep track of the correct operator ordering of the two factors on the RHS of (28). Since in general our method provides wavefunctions of only semiclassical accuracy, the choice of any arbitrary symmetric order will at most lead to corrections of the order of \hbar^2 . Therefore, an obvious choice for the operator version of Ω_5 is

$$\hat{\Omega}_5 = \frac{r}{2x_0} \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial (q_5^1)^2} - \frac{\hbar^2}{2m} \frac{\partial^2}{\partial (q_5^2)^2} + \frac{4Dr^2}{x_0^2} - 8D \right) \frac{r}{2x_0}. \quad (31)$$

The wavefunctions σ_5 , which solve

$$\hat{\Omega}_5 \sigma_5 = 0$$

are then given by

$$\sigma_5(r, \varphi | D, F) = r^{-1} \psi_1(r, \varphi | D, F) \tag{32}$$

where ψ_1 is obtained from (25) after the replacements (30),

$$\begin{aligned} \sigma_5(r, \varphi) = & r^{F/\hbar-1} e^{iF\varphi/\hbar} \int dp \exp[-(2mD)^{1/2}r^2(1+2p)/\hbar x_0] \\ & \times p^{(-1/2+F/2\hbar-(2mD)^{1/2}x_0/\hbar)} (p+1)^{(-1/2+F/2\hbar+(2mD)^{1/2}x_0/\hbar)}. \end{aligned}$$

There arises now the question which value the quantity F should take. In § 4.1 we have shown that F is the value of the angular momentum. Transforming the angular momentum of coordinate system 5 back into coordinate system 1 gives $x_0(-8mq_1^2)^{1/2}$. In order to generate a solution to the Schrödinger equation corresponding to (26) with the energy value $q_1^2 = E$, F has to be

$$F = x_0(-8mE)^{1/2}. \tag{33}$$

If we transform σ_5 with the kernel (29) and make use of (33), we finally obtain

$$\begin{aligned} \sigma_1(q, E) = & \int_0^{2\pi} d\varphi \int_0^\infty r dr \chi^{1+5}(q, E, r, \varphi) \sigma_5(r, \varphi) \\ = & \mathcal{N}(E) \exp[-q(-2mE)^{1/2}/\hbar] \int dp \exp[-(2mD)^{1/2}x_0(2p+1) e^{-q/x_0/\hbar}] \\ & \times p^{(-1/2+(-2mE)^{1/2}x_0/\hbar-x_0(2mD)^{1/2}/\hbar)} \\ & \times (p+1)^{(-1/2+x_0(-2mE)^{1/2}/\hbar+x_0(2mD)^{1/2}/\hbar)}. \end{aligned} \tag{34}$$

This is the exact wavefunction of the Morse system. The energy quantisation of the bound states is obtained again by the requirement that the integrand has no branch point, but a pole at $p = 0$. This holds if

$$E = E_n = -(\hbar^2/2mx_0^2)[-n - \frac{1}{2} + x_0(2mD)^{1/2}/\hbar]^2 \quad \text{with } n = 0, 1, 2, \dots \tag{35}$$

The quantity

$$B = -n - \frac{1}{2} + x_0(2mD)^{1/2}/\hbar = x_0(-2mE)^{1/2}/\hbar$$

corresponds to the quantity F/\hbar in (25). Regularity of ψ_1 and therefore also of σ_5 at $r = 0$ has the effect that the corresponding σ_1 goes to zero exponentially for $q \rightarrow +\infty$, and therefore this leads to normalisability of σ_1 . So, (34) is a regular solution only for $B > 0$, i.e. for

$$n < x_0(2mD)^{1/2}/\hbar - \frac{1}{2}. \tag{36}$$

Accordingly, we obtain only a finite number of regular, single-valued bound state wavefunctions. One notes that (35) is the correct energy quantisation condition of the Morse system. For a conventional treatment of the Morse system see problem 70 in Flügge (1971).

The factor $(-2mE)^{1/2}$ in the exponent of (34) and the corresponding factor $(-8mq_1^2)^{1/2}$ in (27) switches from real to imaginary values on passing from $E > 0$ to $E < 0$. Accordingly, σ_1 decreases exponentially for $q \rightarrow \infty$ if $E < 0$ and becomes oscillatory for $q \rightarrow \infty$ if $E > 0$. The p integral is a modulation function of the plane wavefactor $\exp[-q(-2mE)^{1/2}/\hbar]$. For $q \rightarrow -\infty$ the function σ_1 decreases exponentially for any value of E .

If we insert the second, linearly independent oscillator function (given in (25')) into (32) and the resulting $\tilde{\sigma}_5$ into (34) and perform the same steps as before, then we obtain

$$\begin{aligned} \tilde{\sigma}_1(q, E) = \mathcal{N}(E) \exp[q(-2mE)^{1/2}/\hbar] \int dp \exp[-(2mD)^{1/2}x_0(2p+1) e^{-q/x_0/\hbar}] \\ \times p^{(-1/2-(-2mE)^{1/2}x_0/\hbar-x_0(2mD)^{1/2}/\hbar)} \\ \times (p+1)^{(-1/2-x_0(-2mE)^{1/2}/\hbar+x_0(2mD)^{1/2}/\hbar)}. \end{aligned} \quad (34')$$

We see that the switch from σ_1 to $\tilde{\sigma}_1$ is equivalent to the transition from the positive to the negative branch of the square root in the expressions $(-2mE)^{1/2}$,

The integrand in (34') has a pole at $p=0$ if $-\frac{1}{2}-x_0(-2mE)^{1/2}/\hbar-x_0(2mD)^{1/2}/\hbar$ is a negative integer. This leads to an energy quantisation condition which is identical to (35). This time the quantity

$$\tilde{B} = n + \frac{1}{2} - x_0(2mD)^{1/2}/\hbar = x_0(-2mE)^{1/2}/\hbar,$$

corresponding to the quantity F/\hbar in (25'), has to be negative in order to generate a regular solution, i.e. again we obtain a regular solution only if (36) is fulfilled. Therefore, $\tilde{\sigma}_1$ does not lead to any new bound state solutions.

For positive values of E , $\tilde{\sigma}_1$, given in (34'), is a linearly independent, second solution to the Schrödinger equation of the Morse problem.

4.3.

Now we study the non-relativistic radial hydrogen problem, whose Hamiltonian contains the centrifugal potential $l(l+1)\hbar^2/2mq^2$. In I, § 4.3 we have shown that our transformation method is not able to treat the centrifugal potential correctly. If we transform a Hamiltonian with a centrifugal potential onto a reference Hamiltonian without centrifugal potential, then the reference wavefunction, when transformed back, leads to a Hamiltonian with a modified centrifugal potential, which differs from the original one by terms of the order \hbar^2 . This is because in general the exactness of the composite transformation may not be guaranteed.

Hence, we may start from an initial system with a centrifugal potential modified in such a way that this modification just cancels this error generated by the transformation. As we have shown in I, § 4.3, the appropriate modification is to replace $l(l+1)$ in the original centrifugal potential by $(l+\frac{1}{2})^2$. With this modification the initial problem in coordinate system 1 becomes

$$\Omega_1 = (p)^2/2m - Q^2/q + (l+\frac{1}{2})^2\hbar^2/2m(q)^2 - E. \quad (37)$$

As in the previous example we define $q = q_1^1, p = p_1^1, E = q_1^2, t = p_1^2$. This hydrogen problem is now mapped onto the Morse problem by the following two transformations.

$$F_2^1(q_1, p_2) = -x_0 p_2^1 \ln(q_1^1/x_0) - p_2^2 Q^4/4q_1^2 x_0^2,$$

$$\det \partial^2 F/\partial q_1 \partial p_2 = -Q^4/[4x_0 q_1^1 (q_1^2)^2],$$

$$F_3^2(p_2, q_3) = -p_2^1 q_3^1 + p_2^2 x_0 \ln(2x_0 q_3^2/Q^2) - p_2^2 q_3^2,$$

$$\det \partial^2 F/\partial p_2 \partial q_3 = 1,$$

$$\begin{aligned} \Omega_3 = \{Q^4 \exp(2q_3^1/x_0)/4x_0^2 (q_3^2)^2\}[(p_3^1)^2/2m - 2q_3^2 \exp(-q_3^1/x_0) \\ + q_3^2 \exp(-2q_3^1/x_0) + (l+\frac{1}{2})^2\hbar^2/2mx_0^2]. \end{aligned} \quad (38)$$

This expression within the square brackets coincides with the Morse problem defined by (26), if we make the replacements

$$p \rightarrow p_3^1, \quad D \rightarrow q_3^2, \quad q \rightarrow q_3^1, \quad E \rightarrow -(l + \frac{1}{2})^2 \hbar^2 / 2mx_0^2. \quad (39)$$

Concerning the operator ordering of $\hat{\Omega}_3$ we use the same symmetrisation as in the case of (28) and accordingly the wavefunctions ξ_3 solving $\hat{\Omega}_3 \xi_3 = 0$ are given by

$$\xi_3(q_3) = \exp(-q_3^1/x_0) \sigma_1(q_3^1, -(l + \frac{1}{2})^2 \hbar^2 / 2mx_0^2),$$

where σ_1 is defined by (34),

$$\begin{aligned} \xi_3(q_3) = \mathcal{N}(q_3^2) \exp[-q_3^1(l + \frac{3}{2})/x_0] \int dp (p + 1)^{(l+x_0(2mq_3^2)^{1/2}/\hbar)}, \\ \times p^{(l-x_0(2mq_3^2)^{1/2}/\hbar)} \exp[-x_0(2mq_3^2)^{1/2} \exp(-q_3^1/x_0)(1 + 2p)/\hbar]. \end{aligned} \quad (40)$$

Again, constant factors have been combined into the energy-dependent normalisation factor $\mathcal{N}(q_3^2)$. From (4) and (5) we infer that the transformation kernel is

$$\begin{aligned} \chi^{1-3}(q_1, q_3) = \mathcal{N}(q_1^2)(q_1^1)^{-1/2} \delta(q_3^2 + Q^4/4q_1^2x_0^2) \\ \times \delta(-x_0 \ln(q_1^1/x_0) - q_3^1 + x_0 \ln(2x_0q_3^2/Q^2)), \end{aligned} \quad (41)$$

which leads upon transforming from ξ_3 to ξ_1 to the result

$$\begin{aligned} \xi_1(q, E) = \mathcal{N}(E)q^{l+1} \int dp \exp[q(-2mE)^{1/2}(1 + 2p)/\hbar] \\ \times p^{(l-(-m/2E)^{1/2}Q^2/\hbar)} (p + 1)^{(l+(-m/2E)^{1/2}Q^2/\hbar)}. \end{aligned} \quad (42)$$

This is an exact solution of the radial hydrogen problem with centrifugal potential $l(l + 1)\hbar^2/2mq^2$. Again we obtain the exact energy quantisation by requiring the single valuedness of ξ_1 . The integrand has a pole at $p = 0$ if and only if

$$E = E_\nu = -mQ^4/2\hbar^2(l + \nu + 1)^2 \quad \text{where } \nu = 0, 1, 2, \dots \quad (43)$$

For $E > 0$ a further linearly independent solution ξ_1 can be obtained from ξ_3 if instead of (40) the linearly independent second solution of the Morse problem is used. This leads to the correct hydrogen wavefunction which behaves like q^{-1} at $q = 0$.

5. Conclusions

We have shown, using the examples of the Morse potential and the radial hydrogen problem that the concept of canonical transformations in the extended phase space enables us to treat problems with bound state and continuum spectra along the same lines as in I and II. For the above mentioned two examples the exact integral representations for the wavefunctions resulted and the uniqueness requirement led to the exact energy quantisation.

Let us make three final remarks:

(1) If we do not require exactness of each intermediate transformation kernel, but are satisfied instead with uniform semiclassical kernels in each step, then we can allow for more general transformation generators. We only require that the determinant of the second mixed derivatives factorises into a product of one function of q_k only and

one function of p_{k+1} only. This is sufficient to avoid caustic singularities. If in the final integral for the multistep transformation kernel each step is free of caustic singularities, then it is possible to choose all integration domains in such a way that all integrals converge properly and caustic singularities are never met. Hence a uniformly valid semiclassical approximation for the total transformation kernel is then obtained.

(2) It is not possible to take (12) as a quantisation prescription of the classical variable p_{k+1} , because \hat{p}_{k+1} is not always self-adjoint, especially if non-bijective or complex transformations have been applied. For more details on these objections see II. So, (12) is only a recipe how to correlate a differential operator with p_{k+1} in such a way that the Schrödinger equation transforms in the desired way. In the same spirit, the complete paper may be viewed as a computational recipe, how to construct solutions to a given differential equation, without giving any interpretation of the quantities occurring in intermediate steps.

(3) Example 4.1 raises the following question: can we handle any system with two degrees of freedom by the same method as the two-dimensional oscillator and map any given $H_1(q_1^1, q_1^2, p_1^1, p_1^2)$ onto $H_N = q_N^1$ by an appropriate sequence of canonical transformations? Unfortunately, the answer is no, for the following reason.

The Poisson bracket $\{q_N^1, q_N^2\} = 0$ and therefore q_N^2 is a second conserved quantity in coordinate system N , which is independent of the energy. Then the transformation from q_N^2 back to coordinate system 1 gives a second conserved quantity which commutes with H_1 , because Poisson brackets remain invariant under canonical transformations. It stays independent of energy if the transformations are non-singular. Therefore the system is integrable. However, a generic system with two degrees of freedom is not integrable and it is therefore impossible to map this non-integrable H_1 onto an integrable H_N by a finite sequence of canonical transformations. It is only possible to map a non-integrable H_1 onto another non-integrable H_N . Therefore, the transformation technique as applied in § 4.1 is not suited for generic systems with several degrees of freedom.

At the moment it is not known how to generalise our transformation method to the treatment of non-integrable systems. If it could be done, it would be a big advance, because not much is known about the semiclassical quantisation of non-integrable systems.

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