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Representation of quantum mechanical wavefunctions by complex valued extensions of classical canonical transformation generators

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Abstract. Sufficient conditions are given for the possibility to construct quantum mechanical wavefunctions by the sole knowledge of an appropriate sequence of classical canonical transformations which map a given Hamiltonian onto the new position variable. The transformation matrix element for each individual step of this sequence is given by the semiclassical limit expression of these matrix elements; it is a function of the generator of this transformation step only. The wavefunction, i.e. the transformation matrix element for the total transformation, is obtained as a multiple integral over the transformation matrix elements of the various intermediate steps. The practicability of this procedure is demonstrated by several examples. In this paper we consider time-independent systems with one degree of freedom.

1. Introduction

The equations of classical mechanics are form invariant under canonical transformations. Therefore, we are able to choose in phase space that canonical coordinate system in which the Hamiltonian function of the system under study has the most convenient form. The big advantage of such a choice for investigating mechanical systems is well known. Thus the desire arises to apply canonical transformations in quantum mechanics as well, in order to achieve an analogous simplification of the quantum mechanical Hamiltonian operator. However, the formulation of quantum mechanics is based essentially on a description in Cartesian position and momentum variables and only little is known on how the knowledge of classical canonical transformations can be used in a quantum mechanical treatment.

The important quantities for the quantum mechanical representation of canonical transformations are the scalar products of eigenstates of the old and new position or momentum operators. For the particular transformation which maps the Hamiltonian H onto the new position variable, these matrix elements are the solutions of the Schrödinger equation (see e.g. Miller 1974, § IIC). It is not possible to give these quantum mechanical matrix elements for all canonical transformations in terms of known functions. However, it has been shown by Miller (1974) how all canonical transformations can be handled semiclassically. The semiclassical position matrix elements of that particular transformation, which maps H onto the new position variable, are just the standard WKB approximation for the wavefunctions (see Miller 1974, equation (2.65)). These WKB functions are given as functions of the generator

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of the classical canonical tranformation only. But standard WKB functions are singular at turning points and therefore they are not suited for many applications.

Hence the following question arises: can we improve this and use classical generators to construct wavefunctions which are free of caustics, i.e. uniformly valid, or perhaps even exact wavefunctions? Related to this is the following question; for which class of canonical transformations is it possible to calculate the quantum mechanical matrix elements exactly in terms of known functions? Is it possible to decompose a complicated transformation into a sequence of simple ones, where each member of the sequence is known exactly?

For example, for linear canonical transformations the semiclassical representation is quantum mechanically exact (see Moshinsky and Quesne 1971, Eckelt 1979). But the iteration of linear transformations always results in linear transformations. Therefore, linear transformations are too restricted for building up more complicated transformations. We need a class of canonical transformations fulfilling the following two requirements. (i) They are simple enough, so that the exact quantum mechanical matrix elements are known as functions of the generators. (ii) They must contain nonlinear transformations which, by composition, form more complicated mappings.

The purpose of this paper is to work out these ideas. In § 2 we explain our notation and demonstrate our method of composing a complicated transform from simple ones. In § 3 we derive sufficient conditions for the exactness of semiclassical representations of canonical transformations. Section 4 shows some illustrative examples and § 5 contains final remarks. Throughout, we restrict ourselves to systems with one degree of freedom and to time-independent tranformations.

2. Notation and the composition of canonical transformations in quantum mechanics

Since we study the composition of, say, $N-1$ canonical transforms, defining in the two-dimensional phase space a sequence of N coordinate systems, it is, for the sake of clarity, an indispensable necessity to use a well defined notation. In detail, q_i and p_i are the position and momentum variable in the ith coordinate system. $\hat{q}_i$ and $\hat{p}_i$ are the corresponding quantum mechanical operators. $|q_i(x)\rangle$ and $|p_i(y)\rangle$ are eigenstates of the operators $\hat{q}_i$ and $\hat{p}_i$ with eigenvalues x and y respectively, i.e.

$$\hat{q}_i|q_i(x)\rangle = x|q_i(x)\rangle \qquad \hat{p}_i|p_i(y)\rangle = y|p_i(y)\rangle. \tag{1}$$

The initial coordinate system 1 consists of the standard position and momentum variables and the system under study is described by a Hamiltonian function $H_1(q_1, p_1)$ classically or a Hamiltonian operator $\hat{H}_1(\hat{q}_1, \hat{p}_1)$ quantum mechanically, where $\hat{H}_1 = H_1[x, (\hbar\partial/\mathrm{i})/(\partial/\partial_x)]$ with some ordering prescription.

Let us assume that coordinate system N has the following property. If $\hat{q}_1$ and $\hat{p}_1$ are expressed as functions of $\hat{q}_N$ and $\hat{p}_N$ and inserted into $\hat{H}_1$, then

$$\hat{H}_N(\hat{q}_N, \hat{p}_N) = \hat{H}_1(\hat{q}_1(\hat{q}_N, \hat{p}_N), \hat{p}_1(\hat{q}_N, \hat{p}_N)) = \hat{q}_N. \tag{2}$$

It is evident that the scalar product

$$\psi(x, E) = \langle q_1(x)|q_N(E)\rangle \tag{3}$$

is a solution of the Schrödinger equation

$$H_1\left(x, \frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial x}\right)\psi(x, E) = E\psi(x, E) \tag{4}$$

(see also § IIB in Miller 1974). The scalar product (3) is the position matrix element of the canonical transformation which maps from system 1 to system N. Therefore, in order to find a solution of the Schrödinger equation, it is sufficient to know a way of calculating matrix elements of appropriate canonical transformations. Since it is not possible, in general, to construct an exact solution of the Schrödinger equation in terms of known functions, the same also holds for the exact matrix elements of any complicated canonical transformation. One way to arrive at closed-form expressions for matrix elements of complicated transformations would be to decompose this transformation into a sequence of sufficiently simple ones with exactly known matrix elements. We shall take intermediate steps, for which the exact quantum mechanical matrix elements coincide with the semiclassical expressions. We assume that all intermediate steps are sufficiently close to the identity such that they can be given in terms of generators of type 2 or 3. Without loss of generality we may assume that $N-1$, the number of steps, is even (if not, this can always be achieved by inserting additional identities) and that the various steps are defined by generators of type 2 and 3, alternately.

For shorter notation we use the abbreviations $r = 2l+2$, $r\pm = r \pm 1$ in the following. A transformation from coordinate system $r-$ to coordinate system r is given by the generator $F_2^{r-}(q_{r-}, p_r)$ and the transformation from coordinate system r to coordinate system $r+$ is given by the generator $F_3^r(p_r, q_{r+})$ for all $l \in \{0, 1, \ldots, (N-3)/2\}$. Lower indices denote the type of the generator.

The corresponding semiclassical transformation matrix elements then are (see Miller 1974, equation (2.50), Eckelt 1979, equation (3.25))

$$\varphi^{r-}(x, y) = \langle q_{r-}(x)|p_r(y)\rangle = \left(\frac{1}{2\pi\mathrm{i}\hbar}\frac{\partial^2 F_2^{r-}(x, y)}{\partial x\,\partial y}\right)^{1/2}\exp\left(\frac{\mathrm{i}}{\hbar}F_2^{r-}(x, y)\right) \tag{5a}$$

$$\varphi^{r}(x, y) = \langle p_r(x)|q_{r+}(y)\rangle = \left(\frac{1}{2\pi\mathrm{i}\hbar}\frac{\partial^2 F_3^{r}(x, y)}{\partial x\,\partial y}\right)^{1/2}\exp\left(\frac{\mathrm{i}}{\hbar}F_3^{r}(x, y)\right). \tag{5b}$$

φ is quantum mechanically exact if it satisfies the conditions (see Eckelt 1970, equations (2.13) and (2.14))

$$\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial y}\varphi^{r-}(x, y) = q_r(\hat{q}_{r-}, \hat{p}_{r-})\varphi^{r-}(x, y) \tag{6a}$$

$$y\varphi^{r-}(x, y) = p_r(\hat{q}_{r-}, \hat{p}_{r-})\varphi^{r-}(x, y) \tag{6b}$$

where $\hat{q}_{r-} = x$, $\hat{p}_{r-} = (\hbar/\mathrm{i})(\partial/\partial x)$

$$\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial y}\varphi^{r}(x, y) = -p_{r+}(\hat{q}_r, \hat{p}_r)\varphi^{r}(x, y) \tag{6c}$$

$$y\varphi^{r}(x, y) = q_{r+}(\hat{q}_r, \hat{p}_r)\varphi^{r}(x, y) \tag{6d}$$

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

The composition of an even number of steps always results in a matrix element of two position eigenstates. Therefore, we also need the equations which are fulfilled

by the exact scalar product of two position eigenstates (see Eckelt 1979, equation (2.12)

$$\chi(x, y) = \langle q_{r-}(x) | q_{2k+1}(y) \rangle$$

is exact if

$$\frac{\hbar}{i}\frac{\partial}{\partial y}\chi(x, y) = -p_{2k+1}(\hat{q}_{r-}, \hat{p}_{r-})\chi(x, y) \tag{6e}$$

$$y\chi(x, y) = q_{2k+1}(\hat{q}_{r-}, \hat{p}_{r-})\chi(x, y). \tag{6f}$$

The matrix element for the total transformation is given by

$$\psi(x, E) = \langle q_1(x) | q_N(E) \rangle = \int \mathrm{d}z_2 \ldots \int \mathrm{d}z_{N-1} \langle q_1(x) | p_2(z_2) \rangle$$

$$\times \langle p_2(z_2) | q_3(z_3) \rangle \ldots \langle q_{N-2}(z_{N-2}) | p_{N-1}(z_{N-1}) \rangle \langle p_{N-1}(z_{N-1}) | q_N(E) \rangle. \tag{7}$$

In order to avoid boundary contributions in partial integrations, we choose the integration path in such a way that the integrand vanishes at the endpoints of all paths or that the integration paths are closed in the complex plane. Clearly, the integration paths depend on the boundary conditions for ψ. For the moment we are only interested in finding solutions of equation (4) and do not care about particular boundary conditions. Therefore, we need not specify the integration paths any further at the moment. Details about the choice of integration paths will be given during the discussion of the examples in § 4.

The problem to be investigated now is the following. What are sufficient conditions which the generators of the individual transformation steps have to satisfy, such that the matrix elements of each step (given in equation (5)) solve equations (6*a*)–(6*d*) and that the composite transform (given by equation (7)) fulfils (6*e*) and (6*f*)? A solution to this problem is presented in the following section.

3. Sufficient conditions for finding exact quantum mechanical transforms

Proposition 1. A sufficient condition for equations (6*a*) and (6*b*) or (6*c*) and (6*d*) to be fulfilled by the semiclassical matrix element of equation (5) is that the generator of the transformation is of one of the following forms

$$F_2^{n\to n+1}(q_n, p_{n+1}) = p_{n+1} f(q_n) + g(q_n) \tag{8a}$$

$$F_3^{n\to n+1}(p_n, q_{n+1}) = q_{n+1}\alpha(p_n) + \beta(p_n) \tag{8b}$$

where f, g, α, β are differentiable functions.

We prove this statement for a generator of type 2. The coordinate transformations resulting from generator (8*a*) are

$$q_{n+1} = \frac{\partial F}{\partial p_{n+1}} = f(q_n) \tag{9a}$$

$$p_n = \frac{\partial F}{\partial q_n} = p_{n+1} f'(q_n) + g'(q_n) \qquad p_{n+1} = [p_n - g'(q_n)]/f'(q_n). \tag{9b}$$

A prime always denotes the derivative with respect to the argument of the function.

In order to give the quantum mechanical version of equation (9*b*), we use the ordering prescription

$$\frac{p_n}{f'(q_n)} \to \frac{1}{2}\hat{p}_n \frac{1}{f'(\hat{q}_n)} + \frac{1}{2}\frac{1}{f'(\hat{q}_n)}\hat{p}_n. \tag{10}$$

Then, $\hat{p}_{n+1}$ applied to a function φ of the old position eigenvalue x is given by ($\hat{q}_n = x$, $\hat{p}_n = (\hbar/\mathrm{i})(\partial/\partial x)$

$$\hat{p}_{n+1}\varphi(x) = p_{n+1}(\hat{q}_n, \hat{p}_n)\varphi(x) = [\hat{p}_n - g'(\hat{q}_n)]/f'(\hat{q}_n)\varphi(x)$$
$$= \frac{1}{f'(x)}\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial x}\varphi(x) - \frac{\hbar}{2\mathrm{i}}\frac{f''(x)}{[f'(x)]^2}\varphi(x) - \frac{g'(x)}{f'(x)}\varphi(x).$$

The semiclassical matrix element for transformation (8*a*) is given by equation (5*a*) as

$$\varphi(x, y) = \langle q_n(x) | p_{n+1}(y)\rangle = [f'(x)/2\pi\mathrm{i}\hbar]^{1/2} \exp\{\mathrm{i}/\hbar[yf(x) + g(x)]\}.$$

The function φ has the following properties

$$\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial y}\varphi(x, y) = f(x)\varphi(x, y) = q_{n+1}(\hat{q}_n, \hat{p}_n)\varphi(x, y).$$

Comparison with equation (9*a*) shows that equation (6*a*) is fulfilled.

$$\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial x}\varphi(x, y) = \left(\frac{\hbar}{2\mathrm{i}}\frac{f''(x)}{f'(x)} + yf'(x) + g'(x)\right)\varphi(x, y).$$

Using the ordering prescription (10) we obtain

$$y\varphi(x, y) = \left[\left(\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial x} - g'(x)\right)\Big/ f'(x)\right]\varphi(x, y) = p_{n+1}(\hat{q}_n, \hat{p}_n)\varphi(x, y).$$

Comparison with equation (9*b*) shows that equation (6*b*) is fulfilled. An analoguous proof holds for generator (8*b*) of type 3.

The semiclassical representation of the transformations remains exact if one adds an arbitrary differentiable function $h(p_{n+1})$ on the RHS of equation (8*a*) or a differentiable function $\gamma(q_{n+1})$ on the RHS of equation (8*b*). But it is not necessary to take into account this generalisation because it is always possible to shift any function of the new variable into the generator of the next step of the composite transformation. We take this statement as proposition 2.

Proposition 2.

$$F_2(q_n, p_{n+1}) = p_{n+1}f(q_n) + g(q_n) + h(p_{n+1})$$
$$F_3(p_{n+1}, q_{n+2}) = q_{n+2}\alpha(p_{n+1}) + \beta(p_{n+1})$$

and

$$\tilde{F}_2(q_n, p_{n+1}) = p_{n+1}f(q_n) + g(q_n)$$
$$\tilde{F}_3(p_{n+1}, q_{n+2}) = q_{n+2}\alpha(p_{n+1}) + \beta(p_{n+1}) + h(p_{n+1})$$

lead to the same transform from coordinate system n to coordinate system $n+2$.

Proof. The direct calculation shows that in either case (we use the abbreviation $t=[p_n-g'(q_n)]/f'(q_n)$)

$$p_{n+2}=-\alpha(t) \tag{11a}$$

$$q_{n+2}=[-f(q_n)-h'(t)-\beta'(t)]/\alpha'(t). \tag{11b}$$

A function $\gamma(q_N)$ in the generator of the last step is of no influence on the dependence of q_N on q_{N-1} and p_{N-1}. The function γ can be left arbitrary as long as we only require to map $H_1(q_1, p_q)$ onto q_N. According to (5*b*) and (7) γ produces the factor $\exp\{i\gamma(E)/\hbar\}$ in $\psi(x, E)$. Therefore, $\gamma(q_N)$ can be exploited to normalise the function $\psi(x, E)$ (see example 2 in § 4).

If we compose several steps of the form (8*a*) and (8*b*), then the integral representation (7) of the total transformation is not exact in general. Therefore, it is necessary to deal with still simpler forms of transformations.

Proposition 3. A sufficient condition for equation (7) to provide the exact representation of a composite transformation, if for each step the semiclassical representation is inserted, is that the intermediate steps are given by generators of the following form

$$F_2(q_n, p_{n+1})=a_n p_{n+1}q_n+g_n(q_n) \tag{12a}$$

$$F_3(p_n, q_{n+1})=b_n q_{n+1}p_n+\beta_n(p_n) \tag{12b}$$

where a and b are constants.

Proof by induction. Because (12) is a special case of (8), it is clear that for each step of the composite transformation equations, (6*a*) and (6*b*) or (6*c*) and (6*d*) are fulfilled.

Next we assume that the matrix element for the composition of the first $2l$ steps, given by

$$\chi^{1\to r-}(x, y)=\langle q_1(x)|q_{r-}(y)\rangle=\int \mathrm{d}z_2 \ldots \int \mathrm{d}z_{2l}\langle q_1(x)|p_2(z_2)\rangle \ldots \langle p_{2l}(z_{2l})|q_{r-}(y)\rangle$$

satisfies the following equations $[\hat{q}_1=x,\ \hat{p}_1=(\hbar/\mathrm{i})(\partial/\partial x)]$

$$\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial y}\chi(x, y)=-p_{r-}(\hat{q}_1, \hat{p}_q)\chi(x, y) \tag{13a}$$

$$y\chi(x, y)=q_{r-}(\hat{q}_1, \hat{p}_1)\chi(x, y). \tag{13b}$$

The transformation from coordinate system $r-$ to coordinate system r is given by the generator

$$F_2(q_{r-}, p_r)=a_{r-}q_{r-}p_r+g_{r-}(q_{r-}).$$

Accordingly

$$q_r=a_{r-}q_{r-} \tag{14a}$$

$$p_r=[p_{r-}-g'_{r-}(q_{r-})]/a_{r-}. \tag{14b}$$

The transformation matrix element between coordinate system 1 and coordinate system r is given by equation (7) as

$$\psi(x, z)=\langle q_1(x)|p_r(z)\rangle=\left(\frac{a}{2\pi\mathrm{i}\hbar}\right)^{1/2}\int \mathrm{d}y\,\chi(x, y)\exp\left(\frac{\mathrm{i}}{\hbar}[ayz+g(y)]\right).$$

We find

$$\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial z}\psi(x,z)=\left(\frac{a}{2\pi\mathrm{i}\hbar}\right)^{1/2}\int \mathrm{d}y\, ay\chi(x,y)\exp\left(\frac{\mathrm{i}}{\hbar}[ayz+g(y)]\right)$$

$$=aq_{r-}(\hat{q}_1,\hat{p}_1)\psi(x,z)$$

$$=q_r(\hat{q}_1,\hat{p}_1)\psi(x,z)$$

and

$$z\psi(x,y)=\left(\frac{1}{a2\pi\mathrm{i}\hbar}\right)^{1/2}\int \mathrm{d}y\,\chi(x,y)\left(\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial y}-g'(y)\right)\exp\left(\frac{\mathrm{i}}{\hbar}[ayz+g(y)]\right).$$

Since we assume the path of integration to be such that no boundary contributions arise in integrating by parts, we obtain

$$\left(\frac{1}{a2\pi\mathrm{i}\hbar}\right)^{1/2}\int \mathrm{d}y\,\exp\left(\frac{\mathrm{i}}{\hbar}[ayz+g(y)]\right)\left(-\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial y}-g'(y)\right)\chi(x,y).$$

Using equations (13) we find

$$z\psi(x,y)=\frac{1}{a}[p_{r-}(\hat{q}_1,\hat{p}_1)-g'(q_{r-}(\hat{q}_1,\hat{p}_q))]\psi(x,z)=p_r(\hat{q}_1,\hat{p}_1)\psi(x,z).$$

$\psi(x,z)$ fulfils the partial differential equations, by which the correct transformation matrix element is characterised. Therefore the proposition is valid for the transformation between coordinate systems 1 and r. By analogy one can show that the further transformation step given by a generator of form (12b) results in the exact transformation matrix element for the transformation between coordinate systems 1 and $r+$. Therefore, the exactness of this procedure is shown for any number of steps.

In an indirect way linear transformations fulfil condition (12a) or (12b). The most general linear transformation from coordinate system n to coordinate system $n+1$ is given by the generator (without loss of generality we take a generator of type 2; for a generator of type 3 the argumentations would be analogous)

$$F_2(q_n,p_{n+1})=Aq_n^2+Bq_np_{n+1}+Cp_{n+1}^2+Dq_n+Ep_{n+1}+F$$

where A, B, C, D, E, F are constants. By proposition 2 we can shift the terms Cp_{n+1}^2 and Ep_{n+1} into the next transformation step. The remaining

$$\tilde{F}_2(q_n,p_{n+1})=Bq_np_{n+1}+Aq_n^2+Dq_n+F$$

is of form (12a).

Now we study the composition of two transformation steps given by generators of the form (8a) and (8b). We put $n=1$ in (8a) and $n=2$ in (8b). The composite transforms are given by (11a) and (11b) if we put $n=1$ and $h\equiv 0$. We adopt the following notation

$$\xi(x,z)=\langle q_1(x)|p_2(z)\rangle=(f'(x)/2\pi\mathrm{i}\hbar)^{1/2}\exp\left(\frac{\mathrm{i}}{\hbar}[zf(x)+g(x)]\right)$$

$$\eta(z,E)=\langle p_2(z)|q_3(E)\rangle=(\alpha'(z)/2\pi\mathrm{i}\hbar)^{1/2}\exp\left(\frac{\mathrm{i}}{\hbar}[E\alpha(z)+\beta(z)]\right)$$

$$\psi(x,E)=\int \mathrm{d}z\,\xi(x,z)\eta(z,E). \tag{15}$$

From proposition 1 we know that ξ and η fulfil the following differential equations

$$z\xi(x,z)=\left[\left(\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial x}-g'(x)\right)\Big/f'(x)\right]\xi(x,z)$$

$$=\left(\frac{1}{f'(x)}\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial x}-\frac{\hbar}{2\mathrm{i}}\frac{f''(x)}{[f'(x)]^2}-\frac{g'(x)}{f'(x)}\right)\xi(x,z)$$

$$\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial z}\xi(x,z)=f(x)\xi(x,z)$$

$$E\eta(z,E)=\left[\left(\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial z}-\beta'(z)\right)\Big/\alpha'(z)\right]\eta(z,E)$$

$$=\left(\frac{1}{\alpha'(z)}\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial z}-\frac{\hbar}{2\mathrm{i}}\frac{\alpha''(z)}{[\alpha'(z)]^2}-\frac{\beta'(z)}{\alpha'(z)}\right)\eta(z,E)$$

$$\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial E}\eta(z,E)=\alpha(z)\eta(z,E).$$

Therefore, ψ has the following properties:

$$\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial E}\psi(x,E)=\int \mathrm{d}z\xi(x,z)\alpha(z)\eta(z,E)=\alpha\left[\left(\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial x}-g'(x)\right)\Big/f|'(x)\right]\psi(x,E)$$

$$=-p_3(\hat{q}_1,\hat{p}_1)\psi(x,E).$$

Comparison with (11a) shows that (6e) is fulfilled.

$$E\psi(x,E)=\int \mathrm{d}z\,\xi(x,z)\left(\frac{1}{\alpha'(z)}\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial z}-\frac{\beta'(z)}{\alpha'(z)}-\frac{\hbar}{2\mathrm{i}}\frac{\alpha''(z)}{[\alpha'(z)]^2}\right)\eta(z,E)$$

$$=\int \mathrm{d}z\,\eta(z,E)\left(-\frac{1}{\alpha'(z)}\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial z}+\frac{\hbar}{2\mathrm{i}}\frac{\alpha''(z)}{[\alpha'(z)]^2}-\frac{\beta'(z)}{\alpha'(z)}\right)\xi(x,z).$$

With the abbreviation $s=[(\hbar/\mathrm{i})(\partial/\partial x)-g'(x)]/f'(x)$ we obtain

$$E\psi(x,E)=\left(-\frac{1}{\alpha'(s)}f(x)-\frac{\beta'(s)}{\alpha'(s)}+\frac{\hbar}{2\mathrm{i}}\frac{\alpha''(s)}{[\alpha'(s)]^2}\right)\psi(x,E). \tag{16}$$

Equation (6f) is fulfilled, if (16) leads to

$$E\psi(x,E)=\{[-f(x)-\beta'(s)]/\alpha'(s)\}\psi(x,E). \tag{17}$$

Equation (17) is equivalent to equation (16) if at least one of the following two conditions is fulfilled.

(i) $f(x)=ax$ and the ordering prescription is such that

$$\frac{a\hat{x}}{\alpha'(\hat{s})}=\frac{a}{2}\hat{x}\frac{1}{\alpha'(\hat{s})}+\frac{a}{2}\frac{1}{\alpha'(\hat{s})}\hat{x}=a\frac{1}{\alpha'(\hat{s})}\hat{x}-\frac{\hbar}{2\mathrm{i}}\frac{\alpha''(\hat{s})}{[\alpha'(\hat{s})^2]}.$$

(ii) $\alpha(z)=bz$ so that $\alpha''(z)\equiv 0$ i.e. (17) is fulfilled if either F_2 or F_3 is of the simple form (12).

If both of these conditions are not fulfilled, then the quantum mechanical evaluation of $f(x)/\alpha'(s)$ creates terms containing higher-order derivatives of α and f than the

ones which occur in equation (16). These terms then are of order $\hbar^2$ and of higher order in $\hbar$ (see example 3 in § 4).

A similar calculation shows that the semiclassical composite matrix element of one transformation step of form (8) and several steps of form (12) is still exact.

We can summarise the results of § 3 as follows: A sufficient condition for the matrix element of a canonical transformation to be given exactly by equation (7), where each intermediate step is given by equation (5), can be expressed as follows. At most, one step is of form (8), all other steps are of form (12). If several steps are of form (8), then the error is of order $\hbar^2$ and the composite matrix element of equation (7) is a uniformly valid semiclassical approximation to the exact wavefunction only.

4. Examples

In this section we present a few examples to the statements given in the previous section. For simplicity we restrict ourselves to examples which need two transformation steps only and which can be solved with small effort by conventional methods. So it is easy to compare our results with the standard solutions.

4.1.

A one-dimensional particle moving in a linear potential is an example for which the Hamiltonian

$$H_1(q_1, p_1) = (2m)^{-1}p_1^2 - Kq_1 \tag{18}$$

can be mapped onto $H_3(q_3, p_3) = q_3$ in two steps, whose generators fulfil condition (12).

$$F_2^{1\to 2}(q_1, p_2) = q_1 p_2 \tag{19a}$$

generates the identity transformation and

$$F_3^{2\to 3}(p_2, q_3) = -\frac{1}{6mK}p_2^3 + \frac{1}{K}q_3 p_2. \tag{19b}$$

According to (5) and (7) the position space wavefunction for energy E then is

$$\psi(x, E) = \langle q_1(x)|q_3(E)\rangle = \int \mathrm{d}z\, \langle q_1(x)|p_2(z)\rangle\langle p_2(z)|q_3(E)\rangle$$

$$= \frac{1}{2\pi \mathrm{i}\hbar\sqrt{K}}\int \mathrm{d}z\, \exp\left[\frac{\mathrm{i}}{\hbar}\left(xz + \frac{Ez}{K} - \frac{z^3}{6mK}\right)\right]. \tag{20}$$

The spectrum of p_1 is the entire real axis $\mathbb{R}$ and because of $p_2 = p_1$ we have to integrate z, the eigenvalue of p_2, over the entire real axis. The integrand is oscillatory for $z \to \pm\infty$. However, we could also add the term $-\hbar\varepsilon p_2^2/\mathrm{i}$ to (19*b*) leading to the converging factor $\exp(-\varepsilon z^2)$ in (20) and take the limit $\varepsilon \to 0$ afterwards. Then (20) satisfies all the requirements of §§ 2 and 3.

(20) is an integral representation of the Airy function, which is known to be the exact wavefunction of a linear potential (see Watson 1966, § 6.4).

Stationary phase evaluation of the z integration leads to the standard WKB wavefunction having a caustic singularity at $x = -E/K$. The same WKB function can be obtained by using the generator

$$F_1^{1\to 3}(q_1, q_3) = \frac{1}{3mK}(2mq_3 + 2mKq_1)^{3/2} \tag{21}$$

for the one step transform from H_1 to q_3 in the semiclassical formula for the matrix element $\langle q_1(x)|q_3(E)\rangle$. It is evident that (21) does not fulfil requirement (8). Therefore it is not surprising that it leads to a wavefunction having a turning point singularity.

4.2.

The Hamiltonian

$$H_1(q_1, p_1) = (2m)^{-1}p_1^2 + \tfrac{1}{2}m\omega^2 q_1^2 \tag{22}$$

of the harmonic oscillator can be mapped onto $H_3(q_3, p_3) = q_3$ in two steps, where the first generator is of form (12) and the second one is of form (8). The first transformation with the generator

$$F_2^{1\to 2}(q_1, p_2) = aq_1p_2 + \tfrac{1}{2}\mathrm{i}m\omega q_1^2 \tag{23a}$$

where a is an arbitrary constant, maps H_1 onto

$$H_2(q_2, p_2) = \mathrm{i}\omega p_2 q_2 + a^2 p_2^2/2m.$$

The second transformation with the generator

$$F_3^{2\to 3}(p_2, q_3) = \mathrm{i}q_3 \ln(cp_2)/\omega + a^2 p_2^2/(4\mathrm{i}m\omega) \tag{23b}$$

where c is a constant, then maps H_2 onto q_3. In order to achieve the correct normalisation, we may add to the RHS of (23b) an appropriate function of q_3, $\gamma(q_3)$.

The use of complex extensions of canonical transformations can be motivated along the following lines. For the moment let us shift the term $a^2p_2^2/(4\mathrm{i}m\omega)$ from (23b) into (23a), which is allowed by proposition 2 of § 3. Then (23a) generates a complex linear transformation, which maps H_1 onto $\check{H}_2 = \mathrm{i}\omega p_2 q_2$. $\hat{H}_1$ has a purely discrete spectrum and the lines $H_1(q_1, p_1) = E$ are compact curves (ellipses) in the phase space, whereas $\hat{H}_3$ has a purely continuous spectrum and the lines $H_3(q_3, p_3) = E$ are open curves (straight lines) in the phase space. Because of this change in spectrum the quantum mechanical representation of the transformations which map $\hat{H}_1$ onto $\hat{H}_3$ must not be unitary (see also Leaf 1969). It has been pointed out by Kramer *et al* (1975) that complex linear canonical tranformations are not unitary in quantum mechanics. In addition, an appropriate complex linear transformation can map closed conic sections (ellipses, the curves H_1 = constant) onto open conic sections (hyperbolae, the curves $-\mathrm{i}\check{H}_2/\omega = q_2p_2 = \text{constant}$) and hyperbolae have the same topology as straight lines. Finally, any linear canonical transformation can be handled exactly in quantum mechanics. Therefore, a complex linear transformation is the appropriate first step in order to map ellipses onto straight lines or H_1 onto H_3. The factor i in front of the ln term in (23b) is necessary in order to arrive at a real function H_3 i.e. it is inserted in order to cancel the factor i in $\check{H}_2$.

The wavefunction obtained from generators (23) is

$$\psi(x,E)=\int \mathrm{d}z\,\langle q_1(x)|p_2(z)\rangle\langle p_2(z)|q_3(E)\rangle$$

$$=\frac{\mathrm{e}^{\mathrm{i}\gamma(E)/\hbar}}{2\pi\mathrm{i}\hbar}\int \mathrm{d}z\left(\frac{a\mathrm{i}}{\omega z}\right)^{1/2}\exp\left(\frac{\mathrm{i}}{\hbar}axz-\frac{m\omega x^2}{2\hbar}+\frac{a^2z^2}{4m\omega\hbar}-\frac{E}{\hbar\omega}\ln(cz)\right).$$

To bring this integral into a more familiar form, we perform the variable substitution $z=-2\mathrm{i}s\sqrt{m\hbar\omega}/a$ and set the free constant c to a definite value. The dimension of c should be chosen in such a way that cz is dimensionless and for reasons of a more convenient normalisation we choose $c=\mathrm{i}a(2m\hbar\omega)^{-1/2}$. The integrand then is independent of the constant a.

$$\psi(x,E)=d\exp\left(\frac{\mathrm{i}}{\hbar}\gamma(E)-\frac{m\omega x^2}{2\hbar}\right)2^{-E/2\hbar\omega+1/4}$$

$$\times\frac{1}{2\pi\mathrm{i}}\int \mathrm{d}s\,\exp[2sx(m\omega/\hbar)^{1/2}-s^2]s^{-E/\hbar\omega-1/2}. \tag{24}$$

The constant d combines some unimportant constants.

The first transformation step involves a complex transformation. Therefore, the integration variable z no longer needs to be restricted to the real axis. The integrand in (24) has an essential singularity at infinity and for general values of E a branch point at zero. Besides, the integrand has no singularity and no zeros in the complex plane. A good candidate for the endpoints of the integration path is the point infinity, if the integration path goes to infinity in such a direction that the integrand goes to zero along this path, e.g. along the positive real axis. The integration path must encircle the singularity at the origin. Altogether the following integration path fulfils all requirements. It comes in from infinity along the positive real axis until it has nearly reached the origin. Then the path encircles the origin once and goes back to infinity along the real axis on the next sheet of the Riemannian surface belonging to the branch point at the origin.

For those particular values of E for which $E/\hbar\omega+\frac{1}{2}$ is a positive integer, the branch point turns into a pole and the integration path can be deformed into a circle enclosing the origin. These particular values for E are just the eigenvalues of $\hat{H}_1$.

The exponential function in the integrand of (24) is the generating function for Hermite polynomials. Equation (22.9.17) in Abramowitz and Stegun (1965) gives

$$\exp[2sx(m\omega/\hbar)^{1/2}-s^2]=\sum_k\frac{1}{k!}\mathscr{H}_k[(m\omega/\hbar)^{1/2}x]s^k.$$

For the energy value $E=(n+\frac{1}{2})\hbar\omega$, the s integral in (24) has the value

$$\sum_k\frac{1}{k!}\mathscr{H}_k(m\omega/\hbar)^{1/2}x]\oint\frac{\mathrm{d}s}{2\pi\mathrm{i}}s^{k-n-1}=\frac{1}{n!}\mathscr{H}_n[(m\omega/\hbar)^{1/2}x].$$

Therefore

$$\psi(x,(n+\tfrac{1}{2})\hbar\omega)=d\frac{1}{n!}2^{-n/2}\exp\left(\frac{\mathrm{i}}{\hbar}\gamma((n+\tfrac{1}{2})\hbar\omega)-\frac{m\omega x^2}{2\hbar}\right)\mathscr{H}_n[(m\omega/\hbar)^{1/2}x].$$

To obtain the standard normalisation of the oscillator functions, we choose

$$\exp\left(\frac{\mathrm{i}}{\hbar}\gamma((n+\tfrac{1}{2})\hbar\omega)\right)=\sqrt{n!}\,\frac{1}{d}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}$$

or

$$\gamma(q_3)=\frac{\hbar}{\mathrm{i}}\left\{\frac{1}{2}\ln\Gamma\left(\frac{q_3}{\hbar\omega}+\frac{1}{2}\right)+\ln\left[\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\frac{1}{d}\right]\right\}.$$

After multiplication of both generators (23) by -1 the transformations still map H_1 onto q_3, but now the exponentially exploding wavefunction, containing the factor $\exp(m\omega x^2/2\hbar)$, is created.

4.3.

Next we give an example for the composition of two transformations of form (8) and for its error.

A one-dimensional problem, which is equivalent to the radial problem of the three-dimensional isotropic harmonic oscillator, is given by the Hamiltonian

$$H_1(q_1,p_1)=\frac{p_1^2}{2m}+\frac{m}{2}\omega^2q_1^2+\frac{\hbar^2A^2}{2mq_1^2} \tag{25}$$

where the constant A will be specified later.

The transformation given by the generator

$$F_2^{1\to2}(q_1,p_2)=\mathrm{i}m\omega q_1^2p_2+\tfrac{1}{2}\mathrm{i}m\omega q_1^2+(\hbar/\mathrm{i})A\ln(q_1/x_0) \tag{26a}$$

where x_0 is a constant with the dimension of a length, maps H_1 onto

$$H_2(q_2,p_2)=2\mathrm{i}\omega q_2p_2(1+p_2)+\hbar\omega A(1+2p_2).$$

F_2 is chosen in such a way, that p_2 is dimensionless. The transformation given by the generator

$$F_3^{2\to3}(p_2,q_3)=(\hbar/2\mathrm{i})[(A-q_3/\hbar\omega)\ln p_2+(A+q_3/\hbar\omega)\ln(p_2+1)] \tag{26b}$$

maps H_2 onto $H_3(q_3,p_3)=q_3$.

The corresponding wavefunction, given by (5) and (7) is

$$\psi(x,E)=\mathcal{N}x^{A+1/2}\int \mathrm{d}z\,\exp\left(-\frac{m\omega x^2}{2\hbar}-\frac{1}{\hbar}m\omega x^2z\right)z^{(A/2-1/2-E/2\hbar\omega)}$$
$$\times(z+1)^{(A/2-1/2+E/2\hbar\omega)}. \tag{27}$$

In this example we do not care about normalisation and all constant factors are combined into the unspecified normalisation constant $\mathcal{N}$.

For the z integration in (27) we choose the same integration path as for the s integration in (24).

Direct calculation shows that $\psi(x,E)$ fulfils the differential equation

$$H_1\left(x,\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial x}\right)\psi(x,E)=E\psi(x,E)+\frac{\hbar^2}{8mx^2}\psi(x,E).$$

The last term on the RHS is the error caused by the composition of two transformations whose generators fulfil only (8) but not (12). Even though function (27) is not the exact wavefunction, but only a semiclassical approximation, (27) does not contain the factor $(2mE - m^2\omega^2x^2 - \hbar^2A^2/x^2)^{-1/4}$ which causes the singularities of the primitive WKB function at the turning points. (27) is an integral representation for a confluent hypergeometrical function and this type of function does not have any singularity in the open interval $(0, +\infty)$. Therefore, (27) is a uniform semiclassical approximation to the correct wavefunction.

We can construct the exact wavefunction for Hamiltonian (25) by the following procedure. We take a modified Hamiltonian $\tilde{H}_1$ where A^2 is replaced by $\tilde{A}^2 = A^2 + \frac{1}{4}$ and use the generators (26) with A replaced by $\tilde{A}$. The resulting wavefunction $\tilde{\psi}$ fulfils the differential equation

$$E\tilde{\psi}(x, E) = \left[\tilde{H}_1\left(x, \frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial x}\right) - \frac{\hbar^2}{8mx^2}\right]\tilde{\psi}(x, E) = H_1\left(x, \frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial x}\right)\tilde{\psi}(x, E)$$

i.e. $\tilde{\psi}$ is the exact solution of the Schrödinger equation belonging to the original Hamiltonian H_1 given in (25). Using for A^2 the physical value $l(l+1)$ gives $\tilde{A} = l + \frac{1}{2}$ and

$$\tilde{\psi}_l(x, E) = \mathcal{N}x^{l+1}\exp\left(-\frac{m\omega x^2}{2\hbar}\right)\int \mathrm{d}z\, \exp(-m\omega x^2 z/\hbar) z^{l/2-1/4-E/(2\hbar\omega)} \times (z+1)^{l/2-1/4+E/(2\hbar\omega)}. \tag{28}$$

The branch point of the integrand at $z = 0$ turns into a pole for

$$E = \hbar\omega(2n + \tfrac{3}{2} + l) \tag{29}$$

and $n = 0, 1, 2, \ldots$. These particular E values are the exact eigenvalues of the Hamiltonian $\hat{H}_1$ (see problems 65 and 66 in Flügge 1971).

From (28) we can obtain another integral representation for the wavefunction of the harmonic oscillator given by Hamiltonian (22). The centrifugal term in (25) disappears for $l = 0$ or $l = -1$. According to (28), $l = 0$ leads to functions containing a factor x i.e. to the antisymmetric functions with $\tilde{\psi}(x = 0) = 0$. $l = -1$ leads to the symmetric functions. (29) shows that the choice $l = 0$ leads to the energies $E_n = \hbar\omega(2n + 1 + \frac{1}{2})$ i.e. to the correct energies for odd oscillator states. $l = -1$ leads to the energies $E_k = \hbar\omega(2k + \frac{1}{2})$ i.e. to the correct energies for even oscillator states. (28) gives

$$\tilde{\psi}_0(x, E) = \mathcal{N}x\exp(-m\omega x^2/2\hbar)\int \mathrm{d}z\, z^{-1/4-E/2\hbar\omega}(z+1)^{-1/4+E/2\hbar\omega}\exp(-m\omega x^2 z/\hbar) \tag{30a}$$

$$\tilde{\psi}_{-1}(x, E) = \mathcal{N}\exp(-m\omega x^2/2\hbar)\int \mathrm{d}z\, z^{-3/4-E/2\hbar\omega}(z+1)^{-3/4+E/2\hbar\omega}\exp(-m\omega x^2 z/\hbar). \tag{30b}$$

After the substitution $t = (z + \frac{1}{2})\mathrm{i}m\omega$ of the integration variable, (30) leads to the integral representation of the oscillator functions given by Krüger (1981).

For $\omega = 0$ the Hamiltonian (25) describes the radial problem for a free particle. However, the transformations given by the generators (26) become singular in the

limit $\omega = 0$. In this limit a possible choice for the generators is

$$F_2^{1\to 2}(q_1, p_2) = -q_1^2 p_2 - i\hbar(l+\tfrac{1}{2}) \ln (q_1/x_0) \tag{31a}$$

$$F_3^{2\to 3}(p_2, q_3) = -\frac{mq_3}{2p_2} - i\hbar(l+\tfrac{1}{2}) \ln (p_2/y_0). \tag{31b}$$

These transformations map

$$\tilde{H}_1(q_1, p_1) = (2m)^{-1} p_1^2 + \hbar^2 (l+\tfrac{1}{2})^2/(2mq_1^2)$$

onto q_3. x_0 is a constant with the dimension of a length, y_0 is a constant with the same dimension as p_2. The corresponding wavefunction

$$\xi(x, E) = \mathcal{N} \int \mathrm{d}z\, x^{l+1} z^{l-1/2} \exp\left(-\frac{\mathrm{i}}{\hbar} x^2 z - \frac{\mathrm{i}mE}{2z\hbar}\right)$$

fulfils the differential equation

$$E\xi(x, E) = \left[\tilde{H}_1\left(x, \frac{\hbar}{\mathrm{i}} \frac{\partial}{\partial x}\right) - \frac{\hbar^2}{8mx^2}\right] \xi(x, E).$$

The substitution $s = \mathrm{i}xz(mE/2)^{-1/2}$ leads to a more familiar integral representation of Bessel functions with half integer order

$$\xi(x, E) = \mathcal{N} \sqrt{2mE}\, x \frac{1}{\hbar} \int \mathrm{d}s\, s^{l-1/2} \exp\left(\frac{x}{2\hbar}(s - 1/s)\sqrt{2mE}\right).$$

After multiplication of both generators (31) with -1 the transformations still map H_1 onto q_3. But then the function, which is singular at the origin, is created.

5. Conclusions

We have shown that the quantum mechanical wavefunctions can be constructed as functions of the generators of an appropriate sequence of classical canonical transformations, if these generators fulfil certain requirements. The wavefunction constructed according to equations (5) and (7) is exact, if at most one generator is of form (8) and all other generators are of form (12). If several generators are of form (8) then the wavefunction is not exact but only a semiclassical approximation to the exact one. Even in this case the multistep approximate wavefunction may be better behaved than the primitive WKB function, which corresponds to a one-step transformation of the Hamiltonian onto the new position variable. For example in § 4.3 the error of the multistep wavefunction consists in a shift of the angular momentum value and can be easily removed by starting from a modified Hamiltonian.

In some cases it might also be useful to map H_1 not onto q_N itself but onto some convenient function of q_N and p_N.

In this paper we have treated the simple case of time-independent transformations and one degree of freedom only. The value of the method would be increased significantly by generalising it to time-dependent transformations and to several degrees of freedom. This generalisation will be attempted in a future publication.

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