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Representation of quantum mechanical wavefunctions by transformation generators: II. One-dimensional time-dependent case

C Jung and H Krüger

Fachbereich Physik, Universität, 6750 Kaiserslautern, West Germany

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Abstract. Sufficient conditions are given for constructing 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 kernel for each individual step of this sequence is given by the semiclassical limit expression; it is a function of the generator of this transformation step only. The transformation kernel for the total transformation and the time-dependent wavefunction are obtained as a multiple integral over the product of the transformation kernels of the various intermediate steps. The practicability of this procedure is demonstrated by several examples. In this paper we consider explicitly time-dependent systems with one degree of freedom.

1. Introduction

In a previous paper (Jung and Krüger 1982, hereafter referred to as JK) we have shown how for a time-independent system with one degree of freedom the wavefunction can be obtained in terms of the generators of an appropriate sequence of classical canonical transformations. Now we show how the same method can be applied to explicitly time-dependent systems.

The important quantities for the quantum mechanical representation of time-independent canonical transformations are the scalar products of eigenstates of the old and new position or momentum operators. In general it is not possible to give these transformation matrix elements exactly in terms of known functions. However, it has been shown by Miller (1974) how they can be obtained semiclassically for any canonical transformation. In this approximation the matrix elements are found in terms of the generator of the classical canonical transformation only. In general these matrix elements have caustic singularities at turning points and, therefore, are not suited for many applications.

In JK we have decomposed a given transformation into a sequence of simpler ones and we have derived sufficient conditions so that the resulting semiclassical multi-step transformation matrix element is free of caustic singularities or is exactly even. Here we generalise this technique to time-dependent systems in one degree of freedom. In § 2 we explain the notation and the composition of a complicated transformation from simple ones. In § 3 we derive sufficient conditions for the exactness of the resulting wavefunctions. In § 4 we present some illustrative examples and make some final conclusions in § 5.

2. Notation and the composition of transformations

As far as possible we adopt the notation used in JK. We study the composition of $N-1$ canonical transformations, defining in the two-dimensional phase space a sequence of N coordinate systems. q_i and p_i are the position and momentum variables in the ith coordinate system. In general they are explicitly time-dependent functions of q_{i-1} and p_{i-1}. $\hat{q}_i$ and $\hat{p}_i$ are the corresponding differential operators. The initial coordinate system 1 consists of the standard position and momentum variables. The system under study is described classically by a Hamiltonian function $H_1(q_1, p_1, t)$ or quantum mechanically by a Hamiltonian operator $\hat{H}_1(\hat{q}_1, \hat{p}_1, t)$ where

$$\hat{H}_1 = H_1(x, (\hbar/\mathrm{i})(\partial/\partial x), t) \tag{1}$$

with some ordering prescription. t is the time variable.

Our goal is to transform to a final coordinate system N, in which H has the particularly simple form

$$H_N(q_N, p_N, t) = q_N. \tag{2}$$

In order to obtain sufficiently well behaved semiclassical transformation kernels we decompose the transformation between the coordinate systems 1 and N into a sequence of $N-1$ simple ones. In particular we take intermediate steps, for which the exact quantum mechanical transformation kernels coincide with the semiclassical expressions. Without loss of generality, we may assume that $N-1$, the total number of steps, is even and that the various transformation steps are defined by generators of type two and three alternately. More generally we could choose any sequence of types of generators which fulfils only the following requirement: the new variable in any generator is the same as the old variable in the generator of the following step, but if a transformation is broken into a sequence of simple ones, then the individual steps are close to the identity in most cases and the identity transformation and its neighbourhood is described most easily by generators of type two or three.

For a shorter notation we use the abbreviations $r = 2l+2$, $r\pm = r\pm 1$ in the following. The transformation between coordinate systems $r-$ and r is given by the generator $F_2^{r-}(q_{r-}, p_r, t)$ and the transformation between coordinate systems r and $r+$ is given by the generator $F_3^r(p_r, q_{r+}, t)$. The lower indices denote the type of generator. By analogy with the time-dependent case (see equation (2.80) of Miller (1974) or equation (3.25) of Eckelt (1979)), we define the following semiclassical transformation kernels:

$$\varphi^{r-}(x, y, t) = \left(\frac{1}{2\pi\mathrm{i}\hbar}\frac{\partial^2 F_2^{r-}(x, y, t)}{\partial x\,\partial y}\right)^{1/2} \exp[(\mathrm{i}/\hbar)F_2^{r-}(x, y, t)] \tag{3a}$$

between coordinate systems $r-$ and r, and

$$\varphi^{r}(y, z, t) = \left(\frac{1}{2\pi\mathrm{i}\hbar}\frac{\partial^2 F_3^{r}(y, z, t)}{\partial y\,\partial z}\right)^{1/2} \exp[(\mathrm{i}/\hbar)F_3^{r}(y, z, t)] \tag{3b}$$

between coordinate systems r and $r+$.

In the time-independent case φ is interpreted as the scalar product between the eigenstates of the old and new position or momentum operators. In the time-dependent case this interpretation would not make sense in any case, because $\hat{q}_{r-}$ and $\hat{p}_r$ may be explicitly time-dependent operators. Therefore, the transformation kernel φ is not called a matrix element in this paper.

By analogy with the time-independent case φ is exact if it satisfies the following differential equations:

$$(\hbar/\mathrm{i})(\partial/\partial y)\varphi^{r-}(x, y, t) = q_r(\hat{q}_{r-}, \hat{p}_{r-}, t)\varphi^{r-}(x, y, t) \tag{4a}$$

$$y\varphi^{r-}(x, y, t) = p_r(\hat{q}_{r-}, \hat{p}_{r-}, t)\varphi^{r-}(x, y, t) \tag{4b}$$

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

$$(\hbar/\mathrm{i})(\partial/\partial z)\varphi^{r}(y, z, t) = -p_{r+}(\hat{q}_r, \hat{p}_r, t)\varphi^{r}(y, z, t) \tag{4c}$$

$$z\varphi^{r}(y, z, t) = q_{r+}(\hat{q}_r, \hat{p}_r, t)\varphi^{r}(y, z, t) \tag{4d}$$

where $\hat{q}_r = \mathrm{i}\hbar(\partial/\partial y)$, $\hat{p}_r = y$. The kernel of the transformation which is composed of two steps is given by

$$\chi^{r-\to r+}(x, z, t) = \int \mathrm{d}y\, \varphi^{r-}(x, y, t)\varphi^{r}(y, z, t). \tag{5}$$

χ is exact if it fulfils the differential equations

$$(\hbar/\mathrm{i})(\partial/\partial z)\chi(x, z, t) = -p_{r+}(\hat{q}_{r-}, \hat{p}_{r-}, t)\chi(x, z, t) \tag{4e}$$

$$z\chi(x, z, t) = q_{r+}(\hat{q}_{r-}, \hat{p}_{r-}, t)\chi(x, z, t). \tag{4f}$$

In the same way the transformation kernel composed of n steps is defined by

$$\chi^{1\to n+1}(x, z, t) = \int \mathrm{d}y\, \chi^{1\to n}(x, y, t)\varphi^{n}(y, z, t). \tag{6}$$

A transformation kernel composed of an odd number of steps is exact if it satisfies equations of the type (4*a*) and (4*b*). For an even number of steps equations of the type (4*e*) and (4*f*) must be satisfied.

In order to avoid boundary contributions in partial integrations, we choose the integration paths in equations (5) and (6) in such a way that either the integrand vanishes at the end points or the integration paths are closed loops in the complex plane. Further specification of the paths depends on the boundary conditions for χ. At the moment we are interested only in constructing solutions to the differential equations (4) and do not care about particular boundary conditions.

3. Exactness conditions

Proposition 1. A sufficient condition for equations (4*a*) and (4*b*) or (4*c*) and (4*d*) to be fulfilled by the semiclassical transformation kernels of equation (3) is that the generator of the transformation is of the form

$$F_2^{r-}(q_{r-}, p_r, t) = p_r f(q_{r-}, t) + g(q_{r-}, t) \tag{7a}$$

$$F_3^{r}(p_r, q_{r+}, t) = q_{r+}\alpha(p_r, t) + \beta(p_r, t) \tag{7b}$$

where f, g, α, β are differentiable functions. The proof is exactly the same as in the time-independent case. Therefore, we do not repeat it here (see proof of proposition 1 in JK and insert an additional time dependence into the functions f, g, α, β there).

The semiclassical transformation kernel remains exact if one adds a function $h(p_r, t)$ to the right-hand side of equation (7*a*) or a function $\gamma(q_{r+}, t)$ to the right-hand side of equation (7*b*). It is not necessary to take this generalisation into account because

it is always possible to shift any function of the new variable into the generator of the next step of the composite transformation. This can be shown by direct calculation, exactly as in the time-independent case (see proposition 2 in JK).

A function $\gamma(q_N, t)$ in the generator of the last step does not influence the dependence of q_N on q_{N-1} and p_{N-1}. If γ is independent of time then it does not influence the transformation of $H_{N-1}(q_{N-1}, p_{N-1}, t)$ onto q_N. According to (3) and (6) γ produces the factor $\exp[(\mathrm{i}/\hbar)\gamma(y, t)]$ in $\chi^{1\to N}(x, y, t)$. Therefore γ can be exploited to normalise the function χ.

The composition of several transformation kernels, given by generators of the form (7), according to equations (5) and (6) does not result in the exact transformation kernel of the total transformation. Therefore, it is necessary to deal with even simpler forms of transformations.

Proposition 2. A sufficient condition for equation (6) to provide the exact transformation kernel if the semiclassical transformation kernel is inserted for each step is that the individual steps are given by generators of the form

$$F_2^{r-}(q_{r-}, p_r, t) = a_{r-}(t)p_r q_{r-} + g_{r-}(q_{r-}, t) \tag{8a}$$

$$F_3^{r}(p_r, q_{r+}, t) = b_r(t)p_r q_{r+} + \beta_r(p_r, t) \tag{8b}$$

where a and b are any functions of t. Again the proof is exactly the same as in the time-independent case (see proof of proposition 3 in JK and insert a time dependence into a, b, g, β there).

Exactly as in the time-independent case, it can be shown that for the composition of one transformation step, given by a generator of form (7), with several transformation steps, given by generators of the form (8), the exact transformation kernel is provided by equations (3), (5) and (6). The composition of several transformation steps of form (7) creates an error of order $\hbar^2$ and equation (6) yields a uniform semiclassical transformation kernel.

Up to this step everything has been done in complete analogy to the time-independent case. The main result of this paper is now to show that the composite transformation kernel χ can be used to obtain a solution of the time-dependent Schrödinger equation.

Proposition 3. Let there be a Hamiltonian function $H_1(q_1, p_1, t)$ and a sequence of canonical transformations such that they map H_1 onto $H_N(q_N, p_N, t) = q_N$. At most one transformation step is of form (7); all other transformation steps are of form (8). $\chi^{1\to N}(x, y, t)$ is the corresponding function defined by equations (3) and (6). Then for any value of the constant ε the function

$$\psi(\varepsilon|x, t) = \chi^{1\to N}(x, \varepsilon, t)\exp[-(\mathrm{i}/\hbar)\varepsilon t] \tag{9}$$

is a solution of the Schrödinger equation

$$\mathrm{i}\hbar(\partial/\partial t)\psi(\varepsilon|x, t) = H_1(x, (\hbar/\mathrm{i})(\partial/\partial x), t)\psi(\varepsilon|x, t).$$

To prove this we define a sequence of functions by

$$\psi^N(\varepsilon|z, t) = \exp[-(\mathrm{i}/\hbar)\varepsilon t]\delta(z - \varepsilon) \tag{10a}$$

$$\psi^k(\varepsilon|y, t) = \int \mathrm{d}z\, \varphi^k(y, z, t)\psi^{k+1}(\varepsilon|z, t) \tag{10b}$$

for $k = 1, \ldots, N-1$ and show by induction that

$$i\hbar(\partial/\partial t)\psi^k(\varepsilon|y, t) = H_k(\hat{q}_k, \hat{p}_k, t)\psi^k(\varepsilon|y, t) \tag{11}$$

for any $k \in \{1, \ldots, N\}$ where $\hat{q}_k = y$, $\hat{p}_k = (\hbar/i)\partial/\partial y$ for k odd and $\hat{q}_k = i\hbar\,\partial/\partial y$, $\hat{p}_k = y$ for k even.

$\hat{H}_N = \hat{q}_N$ is the multiplication operator by the position variable and it is evident that

$$i\hbar(\partial/\partial t)\psi^N(\varepsilon|z, t) = \varepsilon\psi^N(\varepsilon|z, t) = z\psi^N(\varepsilon|z, t) = \hat{H}_N\psi^N(\varepsilon|z, t). \tag{12}$$

Assume that ψ^{k+1} fulfils

$$i\hbar(\partial/\partial t)\psi^{k+1}(\varepsilon|z, t) = H_{k+1}(\hat{q}_{k+1}, \hat{p}_{k+1}, t)\psi^{k+1}(\varepsilon|z, t). \tag{13}$$

We have to show that equation (13) implies the validity of equation (11). We assume that k is odd and that the transformation between coordinate systems k and $k+1$ is given by a generator of type two. There is no loss of generality because for even k and for a generator of another type everything would be analogous. For the moment let the generator be of form (7), $F_2^k(q_k, p_{k+1}, t) = p_{k+1}f(q_k, t) + g(q_k, t)$. Accordingly

$$\begin{aligned} q_{k+1} &= \partial F/\partial p_{k+1} = f(q_k, t) \\ p_k &= \partial F/\partial q_k = p_{k+1}f'(q_k, t) + g'(q_k, t). \end{aligned} \tag{14a}$$

$$p_{k+1} = [p_k - g'(q_k, t)]/f'(q_k, t). \tag{14b}$$

Here, and in the following, a prime denotes the derivative with respect to the position variable and a dot denotes the derivative with respect to the time variable. In order to give the quantum mechanical version of (14b) we make use of the ordering prescription

$$\hat{p}_{k+1} = \tfrac{1}{2}\hat{p}_k(f'(\hat{q}_k, t))^{-1} + \tfrac{1}{2}(f'(\hat{q}_k, t))^{-1}\hat{p}_k - (g'(\hat{q}_k, t))/(f'(\hat{q}_k, t)). \tag{15}$$

The corresponding transformation of the Hamiltonian is then

$$\begin{aligned} H_k(q_k, p_k, t) = {} & H_{k+1}(q_{k+1}(q_k, p_k, t), p_{k+1}(q_k, p_k, t), t) \\ & - (\partial F/\partial t)(q_k, p_{k+1}(q_k, p_k, t), t). \end{aligned} \tag{16a}$$

Ordering (15) gives

$$\begin{aligned} \hat{H}_k = {} & H_{k+1}\{f(x, t), [(\hbar/i)(\partial/\partial x) - g'(x, t)]/f'(x, t), t\} \\ & - \dot{f}(x, t)[(\hbar/i)(\partial/\partial x) - g'(x, t)]/f'(x, t) \\ & + (\tfrac{1}{2}i\hbar\dot{f}'(x, t)/f'(x, t)) - \dot{g}(x, t). \end{aligned} \tag{16b}$$

From (10b), (3a) and (13) it follows that

$$\begin{aligned} & i\hbar(\partial/\partial t)\psi^k(\varepsilon|y, t) \\ & = \int dz\,[i\hbar(\partial/\partial t)\varphi^k(y, z, t)]\psi^{k+1}(\varepsilon|z, t) \\ & \quad + \int dz\,\varphi^k(y, z, t)[i\hbar(\partial/\partial t)\psi^{k+1}(\varepsilon|z, t)] \\ & = \int dz\{[\tfrac{1}{2}i\hbar\dot{f}'(y, t)/f'(y, t) - \dot{f}(y, t)z - \dot{g}(y, t)]\varphi^k(y, z, t)\}\psi^{k+1}(\varepsilon|z, t) \\ & \quad + \int dz\,\varphi^k(y, z, t)(\hat{H}_{k+1}(\hat{q}_{k+1}, \hat{p}_{k+1}, t)\psi^{k+1}(\varepsilon|z, t)). \end{aligned} \tag{17}$$

Using $\hat{q}_{k+1} = i\hbar\,\partial/\partial z$, $\hat{p}_{k+1} = z$ and the fact that integration by parts does not cause boundary contributions we obtain for the last term on the right-hand side of (17)

$$\int dz\, \psi^{k+1}(\varepsilon|z, t)(H_{k+1}(-i\hbar\,\partial/\partial z, z, t)\varphi^k(y, z, t)). \tag{18}$$

Because φ^k fulfils equations (4*a*) and (4*b*) this expression can be written as

$$\int dz\, \psi^{k+1}(\varepsilon|z, t)(H_{k+1}(q_{k+1}(\hat{q}_k, \hat{p}_k, t), p_{k+1}(\hat{q}_k, \hat{p}_k, t), t)\varphi^k(y, z, t)).$$

Using equation (4*b*), we note that z in the first term on the right-hand side of (17) acts like

$$p_{k+1}(\hat{q}_k, \hat{p}_k, t) = (\hat{p}_k - g'(\hat{q}_k, t))/f'(\hat{q}_k, t) \qquad \text{where } \hat{q}_k = y,\ \hat{p}_k = (\hbar/i)\,\partial/\partial y.$$

Comparison with (16*b*) shows that equation (17) is equivalent to equation (11). In the same way we can proceed step by step for all k as long as no ordering problems for the operators occur. These ordering problems are the reason that we allow only one generator of form (7). Generators of form (7) lead to fractions of operator functions (see equation (14*b*)) and if we combine several transformation steps, we have to insert several fractions into each other. Then the correct ordering gives rise to higher-order derivatives of the function f than the ones occurring in (17). These additional terms are of order $\hbar^2$ or higher. In addition, the composite transformation kernel $\chi^{1\to N}$ of equation (6) is only correct semiclassically. Therefore, the wavefunction ψ is only a uniform semiclassical solution of the Schrödinger equation if two or more of the transformation steps are given by generators of form (7). Concerning this error compare also the discussion of equations (16) and (17) and example 4.3 in JK. At this point it is appropriate to make a few remarks about equation (15). It is not possible to take equation (15) as a quantisation prescription of the classical variable p_{k+1} because of the following reasons: it is known that a classical observable of the form $\xi(q)p$ is not always quantisable and in particular the operator

$$\tfrac{1}{2}[\xi(\hat{q})\hat{p} + \hat{p}\xi(\hat{q})] \qquad \text{where } \hat{p} = (\hbar/i)(\partial/\partial q)$$

is not always self-adjoint and therefore it does not represent an observable. For a detailed discussion of the problems involved see Wan and Viazminsky (1977) and Wan and McFarlane (1980).

The reason for this violation of self-adjointness of $\hat{p} = (\hbar/i)\,\partial/\partial q$ is a restriction of the range of q; after a non-bijective transformation or a complex-valued transformation the range of q is no longer the entire real axis and hence $\hat{p} = (\hbar/i)\,\partial/\partial q$ can no longer be interpreted straightforwardly as the quantum mechanical operator describing an observable momentum. This is related to the fact that non-bijective transformations or complex-valued transformations cannot be represented quantum mechanically by unitary operators (in this connection see also Leaf 1969 and Kramer *et al* 1975). Under non-unitary transformations the property of an operator to be self-adjoint is not conserved.

Therefore, we adopt the following pragmatical point of view; we do not claim that equation (15) is a quantisation prescription for the classical observable p_{k+1}. It is only a recipe to show how to correlate with p_{k+1} a differential operator 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 on how to construct solutions

to a given differential equation without giving any explanation of the physical meaning of the quantities occurring in intermediate steps.

According to proposition 3 we can construct a solution of the time-dependent Schrödinger equation for any value of the constant ε. The general solution is then given by

$$\psi(x, t) = \int \mathrm{d}\varepsilon\, \psi(\varepsilon|x, t)\zeta(\varepsilon)$$

where $\zeta(\varepsilon)$ is any function of ε. The freedom of choosing any function ζ can be used to solve the Cauchy problem

$$\psi(x, t_0) = \int \mathrm{d}\varepsilon\, \psi(\varepsilon|x, t_0)\zeta(\varepsilon) = \psi_0(x).$$

In some cases it may be more convenient to map a given Hamiltonian H_1 not onto q_N but onto some other convenient function of q_N, p_N and t, which is the Hamiltonian of some reference system. From the proof of proposition 3, it is obvious that our transformation technique can also be applied in this case. We formulate this statement as the following proposition.

Proposition 4. Let there be given a sequence of $k-1$ canonical transformations whose generators are of form (8). These transformations map $H_1(q_1, p_1, t)$ onto $H_k(q_k, p_k, t)$. $\chi^{1\to k}$ is the corresponding transformation kernel according to equations (3), (5) and (6). Let $\xi(y, t)$ be a solution of the Schrödinger equation $\mathrm{i}\hbar(\partial/\partial t)\xi(y, t) = H_k(\hat{q}_k, \hat{p}_k, t)\xi(y, t)$. Then $\psi(x, t) = \int \mathrm{d}y\, \chi^{1\to k}(x, y, t)\xi(y, t)$ satisfies the equation $\mathrm{i}\hbar(\partial/\partial t)\psi(x, t) = H_1(x, (\hbar/\mathrm{i})(\partial/\partial x), t)\psi(x, t)$.

Here we have allowed only for transformation steps of the simple form (8), because in general H_k may be any complicated function of q_k and p_k. If H_k is sufficiently simple, that is, if H_k does not contain any products or fractions of position and momentum operators, then it is possible to allow one step of form (7).

If only semiclassical wavefunctions are desired, then any number of transformation steps of the form (7) may be admitted. In this case it may also be convenient to start from a uniform semiclassical wavefunction of the reference system H_k and to transform it into a uniform semiclassical wavefunction of H_1, the system under investigation.

4. Examples

In this section we present a few examples to illustrate the statements of the previous section. For simplicity we restrict ourselves to examples which can be solved with small effort by conventional methods. So it is easy to compare our solutions with the standard solutions.

4.1.

The driven harmonic oscillator with the Hamiltonian

$$H_1(q_1, p_1, t) = p_1^2/2m + m\omega^2 q_1^2/2 + q_1 K(t) \tag{19}$$

where $K(t)$ is an external time-dependent force. Defining

$$h(t) = \int_{-\infty}^{t} \omega^{-1} \sin(\omega(t-\tau)) K(\tau)\, \mathrm{d}\tau \tag{20}$$

$$g(t) = \int_{-\infty}^{t} [(\dot{h}(\tau))^2 - \omega^2 (h(\tau))^2](2m)^{-1}\, \mathrm{d}\tau \tag{21}$$

the sequence of four transformations with the generators

$$F_2^1(q_1, p_2, t) = q_1 p_2 - q_1 \dot{h}(t) \tag{22a}$$

$$F_3^2(p_2, q_3, t) = -p_2 q_3 + p_2 h(t)/m \tag{22b}$$

$$F_2^3(q_3, p_4, t) = q_3 p_4 + \mathrm{i}m\omega q_3^2/2 - g(t) \tag{22c}$$

$$F_3^4(p_4, q_5, t) = p_4^2/(4\mathrm{i}m\omega) - q_5 \ln(p_4)/\mathrm{i}\omega \tag{22d}$$

transforms the Hamiltonian in the following way:

$$H_2 = p_2^2/2m - p_2 \dot{h}(t)/m + (\dot{h}(t))^2/2m + m\omega^2 q_2^2/2 + q_2 K(t) - q_2 \ddot{h}(t)$$

$$H_3 = p_3^2/2m + m\omega^2 q_3^2/2 + (\dot{h}(t))^2/2m - \omega^2 (h(t))^2/2m$$

$$H_4 = p_4^2/2m + \mathrm{i}\omega q_4 p_4$$

$$H_5 = q_5.$$

Concerning the occurrence of complex-valued transformations, see the discussion of example 4.2 in JK.

Three transformation steps are of form (8) and one step is of form (7). Therefore, we expect to obtain the exact wavefunction from equations (3), (6) and (9), namely

$$\begin{aligned}\psi(\varepsilon|x, t) &= \mathcal{N} \iiint \mathrm{d}\alpha\, \mathrm{d}\beta\, \mathrm{d}\gamma\, \gamma^{-1/2} \exp\{(\mathrm{i}/\hbar)[x\alpha - x\dot{h}(t) - \alpha\beta + \alpha h(t)/m \\ &\quad + \beta\gamma + \mathrm{i}m\omega\beta^2/2 - g(t) + \gamma^2/(4\mathrm{i}m\omega) - \varepsilon \ln(\gamma)/\mathrm{i}\omega - \varepsilon t]\} \\ &= \mathcal{N} \int \mathrm{d}\gamma\, \gamma^{-\frac{1}{2} - (\varepsilon/\hbar\omega)} \exp\{(\mathrm{i}/\hbar)\{-x\dot{h}(t) + \gamma[x + h(t)/m] \\ &\quad + [x + h(t)/m]^2 \mathrm{i}m\omega/2 - g(t) + \gamma^2/(4\mathrm{i}m\omega) - \varepsilon t\}\}. \end{aligned} \tag{23}$$

Since we do not care about normalisation, all unimportant constants are combined into the unspecified normalisation constant $\mathcal{N}$. Because $p_2 = p_1 + h(t)$ and the spectrum of p_1 being the entire real axis, we integrate α, the eigenvalue of p_2, over the entire real axis and similarly because $q_3 = q_1 + h(t)/m$ and the spectrum of q_1 being the entire real axis, we integrate β, the eigenvalue of q_3, over the entire real axis. The third transformation step is complex and therefore the γ integration is not restricted to the real axis. For the γ integration we use the path that comes in from infinity along the positive real axis until it has nearly reached the origin, then encircles the origin once and goes back to infinity along the positive real axis on the next sheet of the Riemann surface of the branch point at the origin of the γ integrand. This integration path is the same as the one used in example 4.2 in JK, which we refer the reader to for more details.

Direct calculation shows that ψ given in (23) is an exact solution of the time-dependent Schrödinger equation. To bring (23) into a more familiar form, we put

$\gamma = -\mathrm{i}2s(m\hbar\omega)^{1/2}$ and obtain

$$\psi(\varepsilon|x,t) = \mathcal{N}\exp[-(x+h(t)/m)^2 m\omega/2\hbar - (\mathrm{i}/\hbar)(x\dot{h}(t)+g(t)+\varepsilon t)]$$
$$\times \int \mathrm{d}s\, s^{-\frac{1}{2}-(\varepsilon/\hbar\omega)} \exp[-s^2 + 2s(x+h(t)/m)(m\omega/\hbar)^{1/2}]. \tag{24}$$

For $\varepsilon = \hbar\omega(n+1/2)$ the s integral is just the Hermite polynomial $\mathcal{H}_n((m\omega/\hbar)^{1/2}(x+h(t)/m))$ (see equation (22.9.17) of Abramowitz and Stegun 1965).

If $\varphi_n(x)$ is the nth eigenfunction of the time-independent oscillator, then

$$\psi((n+1/2)\hbar\omega|x,t) = \varphi_n(x+h(t)/m)\exp[-\mathrm{i}\omega t(n+1/2) - (\mathrm{i}/\hbar)g(t) - (\mathrm{i}/\hbar)x\dot{h}(t)]. \tag{25}$$

This result coincides exactly with the one obtained by Kerner (1958) with conventional methods.

Assuming that $K(t) = 0$ for $t < 0$ and that the initial condition $\psi(x,0) = \psi_0(x)$ is to be fulfilled, where

$$\psi_0(x) = \sum_n a_n \varphi_n(x),$$

then

$$\psi(x,t) = \sum_n a_n \psi((n+\tfrac{1}{2})\hbar\omega|x,t)$$

is the solution of the time-dependent Schrödinger equation with the prescribed initial condition.

4.2.

Time-dependent transformations are best suited to treat problems in which a classical electromagnetic field is coupled to a material system. For an illustrative example let us treat combined gauge and phase transformations within our technique of canonical transformations. This provides examples for canonical mappings from one system to another reference system which can be treated exactly. We study the non-relativistic motion of a particle of charge e in three dimensions. In the particular cases discussed here, the transformations of the various degrees of freedom are independent of each other and the three-dimensional transformation behaves like three independent one-dimensional transformations.

Let the Hamiltonian in the coordinate system 1 be

$$H_1(\boldsymbol{q}_1, \boldsymbol{p}_1, t) = (2m)^{-1}[\boldsymbol{p}_1 - (e/c)(\boldsymbol{A}(\boldsymbol{q}_1,t) - \boldsymbol{\nabla}_{q_1}\Lambda(\boldsymbol{q}_1,t))]^2$$
$$+ e(\varphi(\boldsymbol{q}_1,t) + c^{-1}(\partial/\partial t)\Lambda(\boldsymbol{q}_1,t)) + V(\boldsymbol{q}_1) \tag{26}$$

where $\boldsymbol{A}$ and φ are the potentials of the classical electromagnetic field, and $\Lambda(\boldsymbol{q}_1, t)$ is a function of position and time. Applying the transformation given by the generator

$$F_2^1(\boldsymbol{q}_1, \boldsymbol{p}_2, t) = \boldsymbol{q}_1 \cdot \boldsymbol{p}_2 - (e/c)\Lambda(\boldsymbol{q}_1, t) \tag{27a}$$

removes the Λ-dependent terms in H.

Because we want to transform the old wavefunction in position space representation onto the new wavefunction also in position space representation, we need a sequence of transformations for which the old variable in the first generator and the new variable

in the last generator are both position variables. Therefore, we insert as an intermediate step the identity transformation given by the generator

$$F_3^2(\boldsymbol{p}_2, \boldsymbol{q}_3, t) = -\boldsymbol{p}_2 \cdot \boldsymbol{q}_3 \tag{27b}$$

and obtain the Hamiltonian

$$H_3(\boldsymbol{q}_3, \boldsymbol{p}_3, t) = \tfrac{1}{2}m^{-1}[\boldsymbol{p}_3 - (e/c)\boldsymbol{A}(\boldsymbol{q}_3, t)]^2 + e\varphi(\boldsymbol{q}_3, t) + V(\boldsymbol{q}_3).$$

Both generators are of form (8) and we expect to transform exact wavefunctions onto exact wavefunctions. If $\xi(x, t)$ is a solution of the equation

$$\mathrm{i}\hbar(\partial/\partial t)\xi(\boldsymbol{x}, t) = H_3(\boldsymbol{x}, (\hbar/\mathrm{i})\boldsymbol{\nabla}, t)\xi(\boldsymbol{x}, t)$$

then according to proposition 4 of § 3 the transformed wavefunction is given by

$$\begin{aligned}\psi(\boldsymbol{x}, t) &= \int\int \mathrm{d}\boldsymbol{\alpha}\ \mathrm{d}\boldsymbol{\beta}\ (2\pi\mathrm{i}\hbar)^{-3} \exp\{(\mathrm{i}/\hbar)[\boldsymbol{x}\boldsymbol{\alpha} - (e/c)\Lambda(\boldsymbol{x}, t) - \boldsymbol{\alpha}\boldsymbol{\beta}]\}\xi(\boldsymbol{\beta}, t) \\ &= \exp[-(\mathrm{i}e/\hbar c)\Lambda(\boldsymbol{x}, t)]\xi(\boldsymbol{x}, t).\end{aligned} \tag{28}$$

Direct calculation shows that ψ fulfils the equation

$$\mathrm{i}\hbar(\partial/\partial t)\psi(\boldsymbol{x}, t) = H_1(\boldsymbol{x}, (\hbar/\mathrm{i})\boldsymbol{\nabla}, t)\psi(\boldsymbol{x}, t).$$

4.3.

An interesting special case of a gauge transformation is the transformation by which Reiss (1970) approximately removes the electromagnetic interaction from

$$H_1(\boldsymbol{q}_1, \boldsymbol{p}_1, t) = \tfrac{1}{2}m^{-1}[\boldsymbol{p}_1 - (e/c)\boldsymbol{A}(\boldsymbol{q}_1, t)]^2 + V(\boldsymbol{q}_1). \tag{29}$$

The transformation composed of the generators

$$F_2^1(\boldsymbol{q}_1, \boldsymbol{p}_2, t) = \boldsymbol{q}_1 \cdot \boldsymbol{p}_2 + (e/c)\boldsymbol{q}_1\boldsymbol{A}(\boldsymbol{q}_1, t) \tag{30a}$$

$$F_3^2(\boldsymbol{p}_2, \boldsymbol{q}_3, t) = -\boldsymbol{p}_2 \cdot \boldsymbol{q}_3 \tag{30b}$$

maps H_1 onto

$$H_3(\boldsymbol{q}_3, \boldsymbol{p}_3, t) = \tfrac{1}{2}m^{-1}\left(\boldsymbol{p}_3 + (e/c)\sum_l q_3^{(l)}\boldsymbol{\nabla}_{q_3}A^{(l)}(\boldsymbol{q}_3, t)\right)^2 + (e/c)\boldsymbol{q}_3(\partial/\partial t)\boldsymbol{A}(\boldsymbol{q}_3, t) + V(\boldsymbol{q}_3).$$

Upper indices on q and A are used to indicate vector components. If we apply the correct ordering prescription to the quantum mechanical version of the terms $\boldsymbol{p}_3 \cdot q_3^{(l)}\boldsymbol{\nabla}_{q_3}\boldsymbol{A}^{(l)}(\boldsymbol{q}_3, t)$, then we find precisely the interaction corrections given by equation (12) of Reiss (1970). According to equation (28) the corresponding transformation of the wavefunctions is given by multiplication with the factor $\exp[(\mathrm{i}/\hbar)(e/c)\boldsymbol{x} \cdot \boldsymbol{A}(\boldsymbol{x}, t)]$.

For the special case of a space-independent A, this transformation is the transformation between dipole length and dipole velocity form of the electromagnetic interaction. In this case

$$H_1(\boldsymbol{q}_1, \boldsymbol{p}_1, t) = \tfrac{1}{2}m^{-1}[\boldsymbol{p}_1 - (e/c)\boldsymbol{A}(t)]^2 + V(\boldsymbol{q}_1)$$

is mapped onto

$$H_3(\boldsymbol{q}_3, \boldsymbol{p}_3, t) = \tfrac{1}{2}m^{-1}\boldsymbol{p}_3^2 + (e/c)\boldsymbol{q}_3 \cdot (\partial/\partial t)\boldsymbol{A}(t) + V(\boldsymbol{q}_3)$$

and the wavefunction is transformed according to $\psi(\boldsymbol{x}, t) = \exp(ie/\hbar c)\boldsymbol{x} \cdot \boldsymbol{A}(t))\xi(\boldsymbol{x}, t)$.

5. Conclusions

We have shown that the quantum mechanical wavefunction can be constructed from the generators of an appropriate sequence of classical canonical transformations, if these generators fulfil certain restrictions. The wavefunction obtained according to equations (3), (5) and (6) is exact, if at most one generator is of form (7) and all other generators are of form (8). If several generators are of form (7) then the wavefunction is a uniform semiclassical approximation to the exact one. In this case the multi-step approximate wavefunction is free of caustic singularities in contrast to the primitive WKB function, which corresponds to a one-step transform of the Hamiltonian onto the new position variable.

If we are satisfied with uniform semiclassical wavefunctions, we can even generalise form (7) for the generators and allow for generators of the form

$$F_2(q_n, p_{n+1}, t) = f(q_n, t)h(p_{n+1}, t) + g(q_n, t) + \alpha(p_{n+1}, t)$$

where f, g, h, α are differentiable functions, and similar expressions for generators of the other types. Then the second derivative $\partial^2 F/\partial q_n \partial p_{n+1}$ factorises into a product of one function of q_n only and one function of p_{n+1} only. This avoids the primitive WKB singularities for which it is characteristic that the position of the singularity in one variable depends on the value of the other variable. The typical turning-point singularity is caused by the factor $(E - V(x))^{-1/4}$ in the WKB wavefunction and the position of the singularity in x depends on the E value. If in our multi-step wavefunction each step is free of WKB singularities, then we can choose all integration paths in such a way that all integrals converge properly and hence a uniformly valid semiclassical approximation for the wavefunction is obtained.

In §§ 2 and 3 the theory has been derived for systems with one degree of freedom. In example 4.2 it has been shown how this theory can also be applied to systems with several degrees of freedom as long as the various degrees of freedom are transformed independently of each other.

As mentioned earlier we do not intend to give a physical interpretation of the quantity $\hat{p}_{k+1}$, given in equation (15), within the framework of this paper. The meaning of this quantity is especially unclear in the case of non-bijective transformations and in the case of complex-valued transformations. Therefore, it would be an interesting problem for future work to clarify these questions.

Another problem for future investigations is to develop generalisations of our transformation techniques to non-separable systems with several degrees of freedom and to find transformations which intermix the various degrees of freedom.

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