TIME DEPENDENT COORDINATE TRANSFORMATION FOR SECOND ORDER PARTIAL DIFFERENTIAL EQUATION

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Abstract

The general formalism of time-dependent canonical transformations is applied to the case of coordinate transformations in classical and quantum mechanics. Most of the engineering problems are governed by time-dependent partial differential equations. The spatial derivatives are discretized by the DQM whereas the time derivatives are discretized by low order finite difference schemes.

Keywords: Quantum Mechanics, Canonical Transformation, Quantum Mechanical, Nonlinear Equations

Introduction

The general formalism of time-dependent canonical transformations is applied to the case of coordinate transformations in classical and quantum mechanics. The general scheme of canonical transformations has been displayed in [1]. Here, this formalism is applied to the case of time dependent coordinate transformations of classical and quantum mechanical systems. Equations with variable coefficients, equations in complicated domains, and nonlinear equations cannot, in general, be solved analytically. We shall therefore have an entirely different approach to solving PDEs. The method is based on replacing the continuous variables by discrete variables. Thus the continuum problem represented by the PDE is transformed into a discrete problem in finitely many variables. Naturally we pay a price for this simplification: we can only obtain an approximation to the exact answer, and even this approximation is only obtained at the discrete values taken by the variables.

Coordinate Transformation in Classical Mechanics

Let the open set, $M < R''$ represent the whole position space of a mechanical system. Given another open set $M' < R^n$ and a number of one-to-one mappings gr: $M \to M'$ with the parameter t (the time). For $q \in M$, the functions f and f' are defined by $f(t, q) = g_t(q)$ and $f'(t, q') = g_t^{-1}(q')$ with $f, f'' \in C^{1.}$ With the aid of $f(t, q)$ and $g_t(q)$, canonical transformations can be defined: let

$$F(t, p', q) = \sum_{j=1}^{n} f_j(t, q)\, p'_j + r(t, q) \tag{1.1}$$

be the generating function of the transformation, i.e.

$$q'_j = \frac{\partial F}{\partial p'_j}\,;\;\; p_j = \frac{\partial F}{\partial q'_j} \tag{1.2}$$

In eq. (1.l),f_j denotes the projection on the j-th coordinate of f, i.e. $f\, i = \pi_j\, 0\, f$ and $r(t, q)$ is a real function of C^3 which will be determined below. From eq. (1.2) it follows that the canonical transformation with the generating function F is determined by the coordinate transformation up to derivatives of $r(t, q)$.

From **eq. (1.2)** we have

$$p_j = \sum_{k=1}^{n} \frac{\partial f_k(t, q)}{\partial q_j} p'_k + \frac{\partial r(t, q)}{\partial q_j} = h_j(t, p', q)$$

According to our presumptions, this equation can be solved with respect to p_k

$$p'_k = h'_k\,(t, p, q)$$

Therefore, the transformation G defined by[1])

$$G(t, X) = (t, h'(t, p, q), f(t, q)), \tag{1.3}$$

where $h' = (h'_i, \ldots, h'\pi)$, represents a canonical transformation in the sense that was formulated in [21]. In M', the canonical formalism is induced by $g_t(q)$. The transformation of the position and momentum observables is of particular interest. Let Q_i be the position observable, defined by $Q_i(t, X') = q'_i$ and correspondingly $Q_i(t, X') = q_i$. They both do not depend explicitly on the time t. We then have

$$\begin{aligned} q_i = Q_i(t, X) &= Q_i \circ G^{-1}(t, X') \\ &= Q_i^{(l)}(t, X). \end{aligned} \tag{1.4}$$

Defining the functions

$$Q' = (Q'_1, \ldots, Q'_n) \text{ and } Q^{(l)} = (Q_1^{(l)}, \ldots, Q_n^{(l)})$$ one has

$$\begin{aligned} q_j = \pi_j \circ g_t^{-1}(q') &= \pi_j \circ g_t^{-1}(Q'_1(t, X'), \ldots, Q'_n(t, X')) \\ &= \pi_j \circ g_t^{-1} \circ Q'(t, X'). \end{aligned} \tag{1.5}$$

Comparison of eqs (1.4) and (1.5) yields:

$$Q^{(l)} = g_t^{-1} \circ Q' \tag{1.6}$$

This means that the function Q_i, describing the same measuring equipment as *Qi* in the new (primed) coordinate system, depends on the observables *Q'* as given by eq. (1.6). Similarly, one can discuss the transformation properties of the momentum observable, ending up with an expression which resembles eq. (1.6).

Coordinate Transformations in Quantum Mechanics

We now consider a quantum mechanical system ∑ having the configuration spaces *M* and *M'* with respect to different coordinate systems. It will be shown that there exist unitary operators *V (t)*, which correspond to the classical coordinate transformations *gt(q)* and that, in some sense, the quantum mechanical observables *Pi,Qi* and *P'i, Q'i* are related to each other by the same transformation formula (1.5) and (1.6) as in classical mechanics.

If *M* and *M'* denote the configuration spaces of ∑, it is obvious to use the HILBERT-Spaces $L^2(M)$ and $L^2(M')$, respectively. Defining

$$\omega_t(q) = \left| \frac{\partial(g_t(q))}{\partial(q)} \right|; \quad q \in M$$

we have $\omega_t(q) \neq 0$ for all $q \in M$ as a consequence of our presumption. This enables us to define operators ***V(t)*** for $t \in$ R by

$$(V(t)\,\psi)\,(q') = \omega_t^{-1/2}\big(g_t^{-1}(q')\big)\,e^{i\lambda'(t,q')}\,\psi\big(g_t^{-1}(q')\big) \qquad (1.7)$$

where $\psi \in L^2(M)$, $q' \in M'$ and λ' is an arbitrary (real measurable) function on *M'*. It can easily be shown that *V (t)* is an unitary operator, since it preserves the norm of *y*, is a linear operator and its range is equal to $L^2(M')$.
$X = (p_1, \ldots. p_n; q_1 \ldots \ldots q_n)$

We now proceed to show that the canonical transformation generated by the unitary operator *V(t)* is the quantum mechanical analogue of the classical canonical transformation, generated by *gt(q)*. Let *Qj* and *Qi* be the self-ad-joint position operators and let us define

$$Q_j^{(l)} = V(t)\,Q_j V^*(t) \qquad (1.8)$$

we then have

$$D_{Q_j^{(l)}} = V(t)\,[D_{Q_j}]^2)$$

Now, one can easily verify that

$$Q_j^{(l)} = g_{tj}^{-1}(Q'_1, \ldots, Q'_n) \qquad (1.9)$$

with *Qj* of eq(1.8) and $g^{-1}_{ij} = \pi_j\, g_t^{-1}$ is an operator identity, since the domains of both sides of eq. (9) coincide. Comparing it with eq. (1.6)) eq. (1.9) enables us to conclude that *V(t)* generates a canonical transformation where the position operators have the same transformation properties as in classical mechanics.

A formula for the momentum operators, however, corresponding to eq. (1.9) (thus representing the quantum mechanical analogue of eq. (1.6) for the momentum *P* at first is shown to be valid for a certain class of operators, $P_0 < P$. Let C_0 (*M*) denote the set of all functions which have a compact support in *M* and are r-times continuously differentiable. It is possible to define operators P_0 by $(\partial/\partial q)$ on $C_0(M)$. The operators P_0 are symmetric, and the same holds for P_j in $C_0(M')$. Note that $C_0(M)$ is dense in $L^2(M)$.

Assuming λ' of eq. (1.7) to be differentiable the following theorem holds :

$$V(t)\left[C_0^1(M)\right] = C_0^1(M')$$

Proof: Given a $\psi \in C^1(M)$. By definition we have $(V(t)\,\psi)\,(q') = 0$ if and only if $\psi(g_t^{-1}(q'))=0$, since ω_i and $\exp(i\,\lambda)$ are both nonvanishing functions in *M*. Let *K* be support of ψ and $K'=g_t[K]$. Because of the continuity of g_t, it follows that *K'* is the support of $\psi(g_t\text{-}1(q'))$. Furthermore *K'* is compact since *K*. We thus conclude that *V(t)y* has a compact support, is differentiable (by presumption) and, therefore, lies in $C_0(M')$. Similarly, one proves the inversion, which completes the proof of the above theorem.

Let **us** now focus the discussion on the operator $V(t)P_{0j}\,V^{-1}(t)$. For $\psi \in C^1(M')$, we obtain using eq. (1.7)

$$\left(V(t)\,P_{0j}V^{-1}(t)\psi'\right)(q') = \frac{\hbar}{i}\,\omega_t^{-1/2}\left(g_t^{-1}(q')\right)\frac{\partial}{\partial q_j}\,\omega_t^{1/2}\left(g_t^{-1}(q')\right)\psi'(q')$$
$$-\hbar\sum_l \frac{\partial}{\partial q'_l}\,\lambda'(t,q')\,\frac{\partial g_{tl}(g_t^{-1}(q'))}{\partial q_j}\,\psi'(q')$$
$$+\sum_l \frac{\partial g_{tl}(g_t^{-1}(q))}{\partial q_j}\,(P'_{0l}\psi')\,(q'). \qquad (1.10)$$

Introducing the function $\lambda(t,q)= \lambda'(t, g_t(q))$ and rearranging terms in eq.(1.10) the final result is

$$V(t)\,P_{0j}\,V^{-1}(t) = \frac{1}{2}\sum_l \left[\frac{\partial g_{tl}(g_t^{-1}(Q'))}{\partial q_j},\,P'_{0l}\right]_+ - \hbar\,\frac{\partial\lambda(t,g_t^{-1}(Q'))}{\partial q_j}, \qquad (1.11)$$

in the domain of the 1.h. side of eq. (1.11). On the other hand, the domain of the r.h. side of eq. (1.11) cannot be larger than $C_0(M')$, hence we have that (1.11) is an operator identity. Combining eq. (1.11) with the definition

$$P_{0j}^{(l)} = V(t)\,P_{0j}V^{-1}(t) \qquad (1.12)$$

one obtains the quantum mechanical analogue of eq. (6) for the restricted operators P_0, if the function $r(t,q)$ in eq(1.1) is chosen such that

$$r(t,q) = h\,\lambda(t,q) + s(t) \qquad (1.13)$$

If the symmetric operators P_j and P'_{0j} can be extended to self-ad-joint operators P_j and P_i such that the canonical commutation relations are preserved, (what it the case, e.g., if M and M' are Cartesian products of finite intervals or the whole of R) one can check wether (11) holds with Pj and $P'j$, too.

Conclusion

The most immediate area of interest is the search for a reliable solution technique for the Time Dependent Coordinate Transformation algorithm in two dimensions. Despite the limited success of the Time Dependent Coordinate Transformation method to generate solutions in two dimensions this thesis has presented an interesting solution technique for problems in one dimension. It is obvious though that the method still needs further work and application to other types of problem to test its robustness and suitability for widespread application.

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