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Conservation laws derived by the Neutral-Action Method

A simple application to the Schrödinger equation

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Abstract. Conservation laws are a recognized tool in physical- and engineering sciences. The classical procedure to construct conservation laws is to apply Noether's Theorem. It requires the existence of a Lagrange-function for the system under consideration. Two unknown sets of functions have to be found. A broader class of such laws is obtainable, if Noether's Theorem is used together with the Bessel-Hagen extension, raising the number of sets of unknown functions to three. By using the recently developed Neutral-Action Method, the same conservation laws can be obtained by calculating only one unknown set of functions. Moreover the Neutral Action Method can also be applied in the absence of a Lagrangian, since only the governing differential equations are required for this procedure. In the paper, an application of this method to the Schrödinger equation is presented.

PACS. 11.30.-j Symmetry and conservation laws

1 Introduction

When investigating mathematical problems, the use of conservation laws is common in physical- and engineering sciences for a long time. Some time ago, a broader class of these conservation laws, so-called material conservation laws were established [1]. So far, the literature on these material conservation laws is sparse. One reason might be that it is not always possible to find a physical interpretation of the conservation laws established. But even in that case, conservation laws form a relieable tool for testing new calculation schemes and numerical programming. The classical method in constructing conservation laws, based on Noether's Theorem, can only be applied in certain restricted cases. In her classical approach, Noether (1918) [2] assumed that a Lagrangian function is available for the system of interest. An extension to this method was given by Bessel-Hagen [3]. For both procedures, it is essential that a Lagrangian function is available for the system of interest. Honein et al. [4] developed a procedure in which this requirement is not necessary. By using the recently developed Neutral-Action Method, a given set of governing partial differential equations is sufficient to construct conservation laws. Recently the Neutral-Action-Method was applied successfully to other branches of mechanics [5,6]. An application to quantum mechanics is presented in the following.

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2 Definition of conservation laws

A mechanical system is considered that can be described by a system of q differential equations

$$\Delta_\beta(x_i, \nu_\alpha, \nu_{\alpha,i}) = 0 \qquad \beta = 1, 2, ..., q \tag{1}$$

with

$$\begin{aligned} x_i \qquad & i = 1, 2, ..., m \quad \text{(independent variables)} \\ \nu_\alpha, \nu_{\alpha,i} \qquad & \alpha = 1, 2, ..., \mu \quad \text{(dependent variables)}, \end{aligned}$$

in which the abbreviation $\nu_{\alpha,i}$ stands for $\frac{\partial \nu_\alpha}{\partial x_i}$. If any set of m associated functions

$$P_i \qquad i = 1, 2, ..., m \tag{2}$$

satisfies

$$P_{i,i} = 0 \quad \text{(local formulation)} \tag{3}$$

along solutions of (1), or

$$\int_\Omega P_{i,i}\, \mathrm{d}\Omega = \oint_{\partial\Omega} P_i\, n_i\, \mathrm{d}A = 0 \quad \text{(global formulation)} \tag{4}$$

then $P_{i,i}$ is called a conservation law, P_i being the conserved current.

3 Neutral Action Method

For systems without a Lagrangian, no procedure existed for a systematic construction of conservation laws, until the Neutral Action Method was advanced [4]. All what is required is that the system can be described by a set of differential equations

$$\Delta_\beta(x_i, \nu_\alpha, \nu_{\alpha,i}) = 0. \tag{5}$$

Even if the governing equations can be calculated from a Lagrange function, the application of the Neutral Action Method is useful, since it leads to the same conservation laws in a much simpler way in comparison to Noether's formalism.

First, the concept of a "Null Lagrangian" will be introduced. In the following, let $E_\alpha(\,)$ denote the Euler-operator

$$E_\alpha(\,) = \left[\frac{\partial}{\partial \nu_\alpha} - \frac{d}{dx_i}\left(\frac{\partial}{\partial \nu_{\alpha,i}}\right) + \frac{d^2}{dx_i dx_j}\left(\frac{\partial}{\partial \nu_{\alpha,ij}}\right)\right](\,). \tag{6}$$

If a Lagrange function can be written as $\tilde{L} = dg_i/dx_i = g_{i,i}$ with $g_i = g_i(x_k, \nu_\alpha, \nu_{\alpha,k})$, it can be shown that

$$\tilde{L} = g_{i,i} \Longleftrightarrow E_\alpha(\tilde{L}) = 0 \tag{7}$$

i.e., it satisfies the equation of Euler-Lagrange identically. $\tilde{L}$ is then called a "Null Lagrangian". Setting the variation of the action integral

$$A = \int_\Omega \tilde{L}\, d\Omega \tag{8}$$

of such a Null Lagrangian to zero, one obtains

$$\delta A = 0 \Longleftrightarrow E_\alpha(\tilde{L}) = 0, \tag{9}$$

where δA denotes the variation of the dependent variables. This means that the action integral A does not depend on the explicit functional dependence $g(x)$ inside the domain of integration but only on the values at the boundary of Ω. So the idea is to seek after characteristic functions f_α such that

$$f_\alpha \Delta_\alpha = P_{i,i}. \tag{10}$$

From (7) and (9), it follows

$$E_\beta(f_\alpha \Delta_\alpha) = E_\beta(P_{i,i}) = E_\beta(\tilde{L}) = 0 \Longleftrightarrow \delta \mathrm{A} = 0 \tag{11}$$

with

$$A = \int_\Omega \tilde{L}\, \mathrm{d}\Omega = \int_\Omega f_\alpha \Delta_\alpha\, \mathrm{d}\Omega. \tag{12}$$

The characteristics f_α have to be determined from (11). The action integral behaves neutrally under its variation, so the formalism is called "Neutral Action Method".

4 The Schrödinger-equation

In quantum mechanics, the following equation is associated with a point-wise particle [7]

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = i\hbar\,\frac{\partial \psi}{\partial t}\,, \tag{13}$$

in which

$$\begin{aligned} \nabla^2 &= \text{Laplace-operator} \\ \psi &= \text{wave function} \\ m &= \text{particle mass} \\ V &= \text{potential energy} \\ i = \sqrt{-1} &= \text{complex unity} \\ \hbar = \frac{h}{2\pi} &= \text{reduced Planck's constant.} \end{aligned}$$

Equation (13) is referred to as the Schrödinger-equation. The wave function ψ is connected to the probability density $P(r,t)$ for a particle to be located at point r at time t as follows

$$P(r,t) = |\psi(r,t)|^2. \tag{14}$$

In the following, we are restricting calculations to one dimension. This leads to a more simple mathematical treatment only. All general aspects remain valid. With the notation

$$(\,)' = \frac{\partial}{\partial x}(\,)$$

$$\dot{(\,)} = \frac{\partial}{\partial t}(\,)$$

we can write

$$\Delta = \psi'' - k_1\dot{\psi} - k_2\psi = 0, \tag{15}$$

where

$$k_1 = -i\frac{2m}{\hbar}$$

$$k_2 = \frac{2mV}{\hbar^2}.$$

Consider the classical problem of a finite square-well potential

$$V(x,t) = V_0 > 0 \quad |x| > a \tag{16}$$

$$= \quad 0 \qquad |x| < a \tag{17}$$

as treated in [7]. In this case, k_2 is a constant.

A solution of equation (15) is

$$\psi(t,x) = (C\cos Lx + D\sin Lx)\; e^{-\frac{k_2+L^2}{k_1}t}\,, \tag{18}$$

where C, D and L are arbitrary complex constants.

5 Calculation of conservation laws

The condition for the existence of a conservation law in case of the one-dimensional Schrödinger-equation (15) requires the satisfaction of the equation

$$E(f\Delta) = \left[\frac{\partial}{\partial\psi} - \frac{d}{dx}\left(\frac{\partial}{\partial\psi'}\right) - \frac{d}{dt}\left(\frac{\partial}{\partial\dot{\psi}}\right) + \frac{d^2}{dx^2}\left(\frac{\partial}{\partial\psi''}\right)\right](f\Delta) = 0. \quad (19)$$

Now, we have to specify the dependence of the characteristic f which we take to be

$$f = f(t, x). \quad (20)$$

A simple calculation of equation (19) with (20) results in

$$E(f\Delta) = f'' + k_1\dot{f} - k_2 f = 0. \quad (21)$$

For any f which satisfies its governing equation (21) the associated conserved currents are

$$P_t = f\psi \quad (22)$$

and

$$P_x = \frac{1}{k_1}\left[f'\psi - f\psi'\right], \quad (23)$$

leading to $\dot{P}_t + P'_x = 0$.

In particular, one such f can be found using

$$f(t, x) = g(x)h(t) \quad (24)$$

leading to

$$g'' + K^2 g = 0 \quad (25)$$

and

$$\dot{h} - \frac{k_2 + K^2}{k_1}h = 0 \quad (26)$$

with its solutions

$$g(x) = A\cos Kx + B\sin Kx \quad (27)$$

and

$$h(t) = e^{\frac{k_2+K^2}{k_1}t} \quad (28)$$

here A, B and K are arbitrary complex constants.

The characteristic f follows to be

$$f(t, x) = (A\cos Kx + B\sin Kx)\, e^{\frac{k_2+K^2}{k_1}t}. \quad (29)$$

The characteristic f in equation (29) is similar to the wave-function ψ in equation (18), from which it only differs by the algebraic sign of the exponent of the second term.

The corresponding currents P_t and P_x can now be calculated by equations (22) and (23):

$$P_t = \psi(A\cos Kx + B\sin Kx)\, e^{\frac{k_2+K^2}{k_1}t} \quad (30)$$

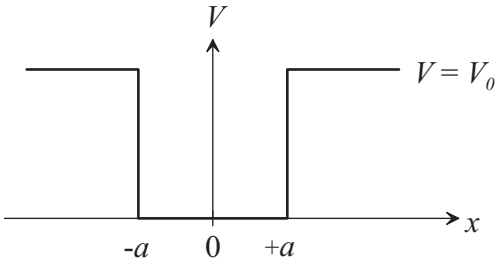

Fig. 1. Static potential.

and

$$P_x = \frac{1}{k_1}\left[K(-A\sin Kx + B\cos Kx)\psi - (A\cos Kx + B\sin Kx)\psi'\right] e^{\frac{k_2+K^2}{k_1}t} \quad (31)$$

in which ψ is already known (18). An interpretation of this conservation law in physical terms is somewhat sophisticated, since it can be looked at as a material conservation law. The notion of material space was established by Eshelby in 1951 [1].

6 Conclusions

The classical procedure of constructing conservation laws is to apply Noether's theorem. It requires the existence of a Lagrangian for the system under consideration. Furthermore, this method demands the knowledge of infinitesimal transformations, which have to be calculated in a separate step. Some further conservation laws can be calculated using the Bessel-Hagen extension, since the equations of motion are left unchanged when a so-called "gauge function" is added to the Lagrangian. In this case, another separate calculation has to be performed. The same conservation laws as above can be obtained by using the Neutral-Action Method, having to calculate only one unknown set of functions f_α. Moreover, the Neutral-Action Method can also be applied in the absence of a Lagrangian, since only the governing equations are required for this procedure. In this present contribution, it is seen that the application of the Neutral-Action Method to quantum mechanic theory has led to novel results. As regards the value and usefulness of conservation and balance laws in a general way, reference may be made to an evaluation of such laws by Olver [8]. It may suffice to mention here the applicability of conservation (and balance) laws in numerics. Being incorporated into various algorithms, the accuracy of the numerical results can be validated by checking whether or not the conservation laws are satisfied identically. If the equations are not satisfied, so-called spurious material nodal forces occur in finite-element calculations, which can be used to improve the finite-element mesh by shifting the nodes in such a way as to eliminate the spurious forces, cf. Herrmann and Kienzler [9], Braun [10], Müller and Maugin [11]. It seems that with a systematic treatment even more conservation laws can be obtained for this problem.

Future work will focus on different forms of the potential energy, especially the non-static case. Studies along this line are in progress and will be dealt with in a forthcoming paper.

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