Force and moment balance equations for geometric variational problems on curves

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We consider geometric variational problems for a functional defined on a curve in a three-dimensional space. The functional is assumed to be written in a form invariant under the group of Euclidean motions. We present the Euler-Lagrange equations as equilibrium equations for the internal force and moment. Examples are discussed to illustrate our approach. This form of the equations particularly serves to promote the study of biofilaments and nanofilaments.

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I. INTRODUCTION

Ever improving experimental techniques in biophysics and nanotechnology have created great interest in onedimensional continuum models for such slender structures as DNA, proteins, nanotubes, and other biofilaments and nanofilaments [1–4]. In addition, such models continue to be used in engineering applications to study large statical deformations of one-dimensional elastic structures (e.g., cables, pipelines, and textile yarns) [5,6]. Vortex filaments provide another target for the application of one-dimensional continuum models [7,8].

Often these models give rise to variational problems on curves in a form that is invariant under Euclidean motions. The corresponding (Euler-Lagrange) equilibrium equations are usually derived *ad hoc*. To be sure, there is a general theory of Euler-Lagrange equations for invariant variational problems [9,10], but it is usually expressed in abstract geometrical form and does not seem to be widely known in the physics and mechanics literature. Moreover, the equations it yields are naturally expressed as high-order ordinary differential equations (ODEs), which are neither necessarily convenient for further analysis or numerical solution nor helpful in providing insight into the problem under consideration.

Here we show that Anderson's Euler-Lagrange equations of [9] for variational problems on curves can be written in the form of (first-order) balance equations for the internal forces and moments in the structure plus equations that can be interpreted as constitutive relations. We believe that this form of the equations is better suited to further analysis, in particular, in problems of rods and filaments subjected to end loads (as, e.g., in single-molecule experiments). We demonstrate the usefulness and wide applicability of the equations by a series of variational problems.

II. EQUATIONS FOR INVARIANT VARIATIONAL PROBLEMS

Consider the variational problem on a smooth curve $C = \{r(s) \in \mathbb{R}^3, s \in [0, L]\}$ for the integral

$$\int_{0}^{L} f[s, \boldsymbol{r}(s), \boldsymbol{\chi}(s)] \mathrm{d}s.$$
 (1)

Here $\chi(s) \in \mathbb{R}^n$ collects possible additional functions defined on the curve. We assume that the functional f is invariant under reparametrizations of the curve C and invariant under the group of Euclidean motions of \mathbb{R}^3 . Then the functional can be expressed in terms of the Euclidean invariant properties of the curve C, i.e., its curvature and torsion. For such problems, it is possible to write down the Euler-Lagrange equations directly in terms of the geometric invariants, i.e., avoiding coordinates r [10]. The following proposition (first briefly announced in [11] in a slightly less general form) gives the equations in the form of force and moment balance equations. The result is a natural convergence of lines of work in mechanics, physics, and mathematics that can be traced back to Sadowsky [12], Langer and Singer [7], Capovilla et al. [13] and, in more abstract form, to the theory of the invariant variational bicomplex [9.10.14].

Proposition. Let $r(s), s \in [0, L]$ be a sufficiently smooth regular curve in \mathbb{R}^3 with unit tangent vector r'(s)=t(s), curvature $\varkappa(s)$, and torsion $\tau(s)$. Here and in the following, the prime denotes differentiation with respect to arclength *s*. In addition, let $\chi(s)$ be a smooth function of arclength. Then the Euler-Lagrange equations for the variational problem

$$\int_0^L f(\boldsymbol{\varkappa}, \boldsymbol{\tau}, \boldsymbol{\chi}, \boldsymbol{\varkappa}', \boldsymbol{\tau}', \boldsymbol{\chi}', \boldsymbol{\varkappa}'', \boldsymbol{\tau}'', \boldsymbol{\chi}'', \dots, \boldsymbol{\varkappa}^{(p)}, \boldsymbol{\tau}^{(q)}, \boldsymbol{\chi}^{(r)}) \mathrm{d}s \quad (2)$$

can be presented in the form of (a) balance equations for the components of the internal force $\mathbf{F} = (F_t, F_n, F_b)^T$ and moment $\mathbf{M} = (M_t, M_n, M_b)^T$ expressed in the Frenet frame $\{t, n, b\}$ (tangent, principal normal, and binormal),

$$\mathbf{F}' + \boldsymbol{\omega} \times \mathbf{F} = \mathbf{0}, \quad \mathbf{M}' + \boldsymbol{\omega} \times \mathbf{M} + \mathbf{t} \times \mathbf{F} = \mathbf{0},$$
 (3)

where $\boldsymbol{\omega} = (\tau, 0, \varkappa)^T$ is the strain (Darboux) vector in the Frenet frame, (b) the "constitutive" equations

$$M_b = \mathcal{E}_{\varkappa}(f), \quad M_t = \mathcal{E}_{\tau}(f), \tag{4}$$

and (c) the equations

$$\mathcal{E}_{\chi_i}(f) = 0, \quad i = 1, 2, \dots, n,$$
 (5)

with \mathcal{E}_{ζ} as the Euler-Lagrange operator for the variable ζ defined by $\mathcal{E}_{\zeta}(h) = \partial_{\zeta} h - (\partial_{\zeta'} h)' + (\partial_{\zeta''} h)'' - \dots$

Note. We adopt the notation that for any vector $\boldsymbol{v} \in \mathbb{R}^3$ the

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triple of components $(v_t, v_n, v_b) = (v \cdot t, v \cdot n, v \cdot b)$ is denoted by the sans-serif symbol **v**. Equation (3) in vectorial form reads as F' = 0, $M' + r' \times F = 0$, the familiar balance equations for a one-dimensional elastic continuum [15]. It follows that F and $M + r \times F$ are constant vectors in space and that $|\mathbf{F}|$ and $\mathbf{F} \cdot \mathbf{M}$ are first integrals.

Proof. It was proven by Anderson [9] by performing the variation of the curve that the Euler-Lagrange equations for \varkappa and τ for the problem in Eq. (2) are given by

$$\varkappa \mathcal{H} + (\varkappa^2 - \tau^2) \mathcal{E}_{\varkappa} + \mathcal{E}_{\varkappa}'' + 2\varkappa \tau \mathcal{E}_{\tau} + \left(\frac{\varkappa \tau' - 2\tau \varkappa'}{\varkappa^2}\right) \mathcal{E}_{\tau}' + 2\frac{\tau}{\varkappa} \mathcal{E}_{\tau}''$$
$$= 0, \qquad (6)$$

$$\tau' \mathcal{E}_{\varkappa} + 2\tau \mathcal{E}_{\varkappa}' - \varkappa' \mathcal{E}_{\tau} + \left(\frac{\varkappa^2 (\tau^2 - \varkappa^2) - 2\varkappa'^2 + \varkappa\varkappa''}{\varkappa^3}\right) \mathcal{E}_{\tau}' + 2\frac{\varkappa'}{\varkappa^2} \mathcal{E}_{\tau}'' - \frac{1}{\varkappa} \mathcal{E}_{\tau}''' = 0,$$

$$(7)$$

where $\mathcal{H} = \mathcal{H}(f)$ is the Hamiltonian

$$\mathcal{H}(f) = -f + \sum_{p \ge i > j \ge 0} \varkappa^{(i-j)} (-1)^j \frac{\mathrm{d}^j}{\mathrm{d}s^j} \left(\frac{\partial f}{\partial \varkappa^{(i)}}\right)$$
$$+ \sum_{q \ge i > j \ge 0} \tau^{(i-j)} (-1)^j \frac{\mathrm{d}^j}{\mathrm{d}s^j} \left(\frac{\partial f}{\partial \tau^{(i)}}\right)$$
$$+ \sum_{k=1}^n \sum_{r \ge i > j \ge 0} \chi_k^{(i-j)} (-1)^j \frac{\mathrm{d}^j}{\mathrm{d}s^j} \left(\frac{\partial f}{\partial \chi_k^{(i)}}\right). \tag{8}$$

Equation (5) is nothing but the set of standard Euler-Lagrange equations for the functions χ_i . We now show that Eqs. (3) and (4) are simply a rearrangement of Eqs. (6) and (7). Consider first the equation for the moment in Eq. (3) and rewrite it in component form,

$$M_t' - \varkappa M_n = 0, \tag{9}$$

$$M_n' - \tau M_b + \varkappa M_t = F_b, \tag{10}$$

$$M_b' + \tau M_n = -F_n. \tag{11}$$

Equation (9) with the help of the second equation in Eq. (4) allows us to express the principal normal component as

$$M_n = \mathcal{E}'_{\tau} / \varkappa. \tag{12}$$

This component of the moment, together with the two components in Eq. (4), we insert into Eqs. (10) and (11) to find

$$F_n = -\mathcal{E}'_{\varkappa} - \frac{\tau}{\varkappa} \mathcal{E}'_{\tau},\tag{13}$$

$$F_b = -\tau \mathcal{E}_{\varkappa} + \varkappa \mathcal{E}_{\tau} + \left(\frac{\mathcal{E}_{\tau}'}{\varkappa}\right)'. \tag{14}$$

Next, we turn to the force equation in Eq. (3), which in component form reads as

$$F_t' - \varkappa F_n = 0, \tag{15}$$

$$F_n' - \tau F_b + \varkappa F_t = 0, \tag{16}$$

$$F_b' + \tau F_n = 0. \tag{17}$$

Now, it follows directly from Eq. (8) that

$$\mathcal{H}' = -\varkappa' \mathcal{E}_{\varkappa} - \tau' \mathcal{E}_{\tau} \tag{18}$$

[here we have used that $\mathcal{E}_{\chi}=0$, by Eq. (5)], and if we combine Eq. (18) with Eqs. (15) and (13) and integrate, we obtain

$$F_t = -\mathcal{H} - \varkappa \mathcal{E}_{\varkappa} - \tau \mathcal{E}_{\tau} + \text{const.}$$
(19)

The integration constant is fixed by the boundary conditions through the integral $|\mathbf{F}|$ and can be absorbed into the Hamiltonian \mathcal{H} . This defines all the force and moment components, and the two equations that have not been used yet [Eqs. (16) and (17)], after substitution of the force components from Eqs. (13), (14), and (19), yield Eqs. (6) and (7).

It is clear that the above steps can be carried out in the opposite direction, i.e., by formally introducing new variables F_t , F_n , F_b , M_t , M_n , and M_b according to the above expressions one can write Eqs. (6) and (7) as a first-order system. Therefore, Eqs. (3) and (4) are equivalent to Eqs. (6) and (7).

A few remarks are in order:

(i) Equations (3) and (4) can be thought of as arising in two steps. In the first step, f is viewed as a function of independent variables \varkappa and τ , and Eq. (4) are the classical Euler-Lagrange equations with M_h and M_t playing the role of generalized forces. The order of derivatives in the operators \mathcal{E}_{\varkappa} and \mathcal{E}_{τ} is determined by the order of derivatives of \varkappa and τ appearing in f. The second step then is to realize that \varkappa and τ are not arbitrary variables, but in fact the curvature and torsion of a space curve. Equation (3) or equivalently Eqs. (6) and (7) are then the result of expressing the variations of \varkappa and τ in terms of variations of the curve *r*. Since curvature is expressed as the second derivative of r and torsion as the third derivative of r, Anderson's equations involve derivatives up to order 2 in \mathcal{E}_{\varkappa} and up to order 3 in \mathcal{E}_{τ} . The balance equations in Eq. (3) are a rewrite of these equations as a first-order system. The components of \mathbf{M} couple the equations of step one to those of step two.

(ii) The reason for calling Eq. (4) constitutive equations is that it is these equations that contain the physics of the problem [the balance equations in Eq. (3) do not depend on fexplicitly]. Writing the Euler-Lagrange equations in the form of Eqs. (3)–(5) is a way of extracting constitutive equations from the functional f. Mathematically, Eq. (4) is best viewed as equations for \varkappa and τ , although they need not be resolved for the highest derivatives of these variables.

(iii) Equivalents of Eqs. (6) and (7) have been derived many times in the literature for particular applications. Examples include the isotropic Kirchhoff rod [7], the Helfrich rod [16] (corrected in [17]), piezoelectric nanobelts [18], magnetic vortex filaments [8], functionals that involve either curvature or torsion or both [13], a functional that depends on curvature only [1], the Sadowsky functional for a narrow developable strip [19], a functional that depends on \varkappa , τ , and their first derivatives [20], a functional that involves \varkappa , τ , χ_1 , and χ'_1 [2], etc. However, the explosion of terms that occurs when \mathcal{E}_{\varkappa} and \mathcal{E}_{τ} are substituted makes Eqs. (6) and (7) not particularly practical either for analytical or numerical study (for all but the very simplest functionals f).

(iv) It may happen that the right-hand sides in Eq. (4) have a simpler form in some other variables and accordingly we may prefer to rewrite Eq. (4) [and Eq. (5)] in these new terms. Let the transformation be given by

$$\begin{split} \xi &= \xi(\varkappa, \tau, \chi, \varkappa', \tau', \chi', \varkappa'', \tau'', \chi'', \ldots), \\ \xi^{(i)} &= \frac{\mathrm{d}^{(i)}\xi}{\mathrm{d}s^{(i)}}, \quad i = 1, 2, \ldots, \\ \eta &= \eta(\varkappa, \tau, \chi, \varkappa', \tau', \chi', \varkappa'', \tau'', \chi'', \ldots), \\ \eta^{(i)} &= \frac{\mathrm{d}^{(i)}\eta}{\mathrm{d}s^{(i)}}, \quad i = 1, 2, \ldots. \end{split}$$

Then the Euler-Lagrange operators are transformed by [21]

$$\mathcal{E}_{\varkappa}(f) = \sum_{i=0}^{\infty} (-1)^{i} \frac{\mathrm{d}^{i}}{\mathrm{d}s^{i}} \left[\frac{\partial \xi}{\partial \varkappa^{(i)}} \mathcal{E}_{\xi}(\tilde{f}) + \frac{\partial \eta}{\partial \varkappa^{(i)}} \mathcal{E}_{\eta}(\tilde{f}) \right], \quad (20)$$

$$\mathcal{E}_{\tau}(f) = \sum_{i=0}^{\infty} (-1)^{i} \frac{\mathrm{d}^{i}}{\mathrm{d}s^{i}} \left[\frac{\partial \xi}{\partial \tau^{(i)}} \mathcal{E}_{\xi}(\tilde{f}) + \frac{\partial \eta}{\partial \tau^{(i)}} \mathcal{E}_{\eta}(\tilde{f}) \right], \quad (21)$$

where \tilde{f} is the transformed f (similar expressions hold for χ as in the usual case of Lagrangians involving higher-order derivatives).

III. EXAMPLES

We illustrate the above theory by several examples.

The anisotropic Kirchhoff rod [7]. Let the curvature $\varkappa(s)$ and torsion $\tau(s)$ define the centerline $\mathbf{r}(s)$ of the rod (up to Euclidean motions). Assuming a noncircular cross-section with bending stiffnesses A and B and torsional stiffness C, we can write the elastic energy density as [22]

$$f(\varkappa,\tau,\phi,\phi') = (a+b\,\cos\,2\phi)\varkappa^2 + c(\tau+\phi')^2,\qquad(22)$$

where a = (A+B)/4, b = (B-A)/4, c = C/2, and ϕ is the twist angle describing the rotation of the local material frame with respect to the Frenet frame about the tangent vector t=r'. With ϕ playing the role of χ_1 , Eqs. (4) and (5) then give, respectively,

$$M_b = \partial_{\varkappa} f = 2(a+b\,\cos\,2\phi)\varkappa,\tag{23}$$

$$M_t = \partial_\tau f = C(\tau + \phi') \tag{24}$$

$$c(\tau' + \phi'') + b\varkappa^2 \sin 2\phi = 0.$$
 (25)

Equations (3) and (23)–(25) constitute a system of differential-algebraic equations (DAEs) that can be turned into a system of ODEs by the differentiation of the algebraic

and

equations. For an isotropic rod (A=B), the coefficient *b* vanishes and a combination of Eqs. (25) and (24) gives the first integral $M_i =: \overline{c} = \text{const}$, which allows the system to be integrated in closed form. In this case, the equation for the angle ϕ fully decouples from the other equations and the centerline of the isotropic rod can be found as a minimizer of the functional $f = ax^2 + \overline{c}\tau$ with a linear torsion term [7]. On the other hand, the functional $f = \frac{1}{2}Ax^2 + \frac{1}{2}C\tau^2$ with quadratic torsion was proposed to model elastic strips and polymer chains [23,24]. It may be formally obtained from Eq. (22) by pushing one of the bending stiffnesses *B* to infinity (implying $\phi \rightarrow \pi/2$). Rods described by this functional bend only about a single principal axis and therefore have their material frame locked to the Frenet frame.

For a bundle of parallel thin rods of circular cross-section of radius R, the normalized bending energy density may be shown to equal [25]

$$f = (1 - \sqrt{1 - R^2 \varkappa^2}), \tag{26}$$

which provides another example of an invariant functional [26]. Grason [27] gives extensions to more complicated functionals for parallel bundles to which our proposition can be applied to derive equilibrium equations.

The Helfrich rod. In order to study chiral effects in polymers, Helfrich proposed the following elastic energy density with higher-order terms included [3]:

$$f = f(\varkappa, \tau, \varkappa') = \frac{k_2}{2}\varkappa^2 + k_3\varkappa^2\tau + \frac{k_{22}}{4}\varkappa^4 + \frac{k_4}{2}(\varkappa'^2 + \varkappa^2\tau^2),$$
(27)

where k_2, k_3, k_{22}, k_4 are constant coefficients. For this functional, Eq. (4) becomes

$$M_{b} = k_{2}\varkappa + 2k_{3}\varkappa\tau + k_{22}\varkappa^{3} + k_{4}\varkappa\tau^{2} - k_{4}\varkappa'', \qquad (28)$$

$$M_t = k_3 \varkappa^2 + k_4 \varkappa^2 \tau. \tag{29}$$

These are the nonlinear constitutive equations for the Helfrich rod (expressed in the Frenet frame). The second equation is algebraic and can be used to eliminate the torsion τ . The first equation is then a differential equation for \varkappa that is to be solved in conjunction with the balance equations. The Helfrich functional has been extended to the sixth order, involving the first derivative of torsion and the second derivative of curvature [28].

A rod lying in a surface. The proposition can also be used in problems of curves with constraints such as the constraint for a rod to lie in a surface. If this surface constraint is given by the pointwise condition $0=g(\varkappa, \tau, \psi, \varkappa', \tau', \psi', ...) \in \mathbb{R}^m$, $\psi \in \mathbb{R}^{m-1}$, for certain *m*, then we consider the new functional $f+\lambda(s) \cdot g$ with $\lambda(s) \in \mathbb{R}^m$ as a Lagrange multiplier.

The simplest example is that of a rod in a *plane*. One may constrain the centerline r=(x, y, z) to a plane by imposing, for instance, z=0, as in [29], but this constraint is not Euclidean invariant and therefore not of the type g above. A Euclidean invariant form is simply $\tau=0$. We can account for this constraint by modifying the function in Eq. (22) and considering $f_1=f+\lambda(s)\tau$ (hence $\chi_1=\phi, \chi_2=\lambda$). Equation (23) does not change while Eq. (24) now becomes $M_t=C(\tau)$

 $+\phi')+\lambda$ and may be used to find the reaction λ . The binormal force component is constant by virtue of Eq. (17). The remaining five Eqs. (15), (16), and (9)–(11) plus Eq. (25) with $\tau=0$ and \varkappa substituted from Eq. (23) form a system of six differential equations for the six variables $M_{t}, M_{n}, M_{b}, F_{t}, F_{n}, \phi$.

Note that the reaction λ has the interpretation of a moment about the tangential direction. The constraint may therefore be realized by applying a distributed twisting couple of the same magnitude. It may be approximated by a rod with multiple (in the limit distributed) small whiskers perpendicular to the centerline (not unlike a caterpillar). If we imagine placing such a hairy rod between two parallel friction-free plates so that the rod itself would not get in touch with the plates then the normal reaction forces would give the required couples.

This way of realizing the constraint differs of course from the usual one corresponding to the z=0 condition, where the reactions are distributed normal *forces* exerted by the plates onto the rod [29]. Anyway, if one is only interested in the configuration of the rod then the realization of the constraint does not matter. In particular, for the isotropic rod the equations in both cases reduce to those of the Euler elastica, \varkappa'' $+\frac{1}{2}\varkappa^3=0$, corresponding to the functional $f=\varkappa^2$.

The Helfrich rod can be similarly constrained to the plane by introducing the condition $\tau=0$. A more direct way to obtain the reduced functional is to delete the torsion terms in the right-hand side of Eq. (27) to obtain $f=\frac{1}{2}k_2\varkappa^2+\frac{1}{4}k_{22}\varkappa^4$ $+\frac{1}{2}k_4\varkappa'^2$ and consider the problem in \mathbb{R}^2 . This functional may be useful for studying polymers synthesized at the interface of two fluids. It may also have an application in computer vision. In this field, the functional $f=\varkappa'^2$ has been proposed for shape completion [30]. The Euler-Lagrange equation for this functional, $\varkappa''''+\varkappa^2\varkappa'-\frac{1}{2}\varkappa\varkappa'^2=0$, follows directly from Anderson's Eq. (6) [9] (the equation in [30] is incorrect). Functionals that involve the torsion may be of interest when one deals with the completion of space curves reconstructed from their planar projections.

Rods confined to a *cylinder* are relevant for buckling inside tubes and for supercoiled filaments and have been studied by imposing the coordinate constraint $x^2+y^2=R^2$, where *R* is the radius of the cylinder [5]. A Euclidean invariant form of the constraint involves two conditions [31],

$$g_1 \coloneqq \varkappa^2 - \varkappa_0^2 \cos^4 \theta - \theta'^2 = 0,$$

$$g_2 \coloneqq \varkappa \theta' - \varkappa' \theta' + \varkappa_0 \varkappa \cos^2 \theta(\varkappa_0 \sin \theta \cos \theta - \tau) = 0,$$
(30)

where $\varkappa_0^{-1} = R$ and $\theta(s)$ is an unknown function that is to be found as part of the solution. The modified functional f $+\lambda_1(s)g_1+\lambda_2(s)g_2$ is of the required form in Eq. (2) (with $\chi_1=\lambda_1, \ \chi_2=\lambda_2, \ \chi_3=\theta$) and the Euler-Lagrange equations follow from the proposition.

Inextensible strips. An inextensible strip is a thin shell that deforms by pure bending (no stretching). Its surface is therefore developable and has a single nonzero principal curvature \varkappa_1 . The normalized bending energy for a rectangular strip of length *L* and width 2w can be reduced to a single integral over the strip's centerline [32,6],

$$\int_{0}^{L} \int_{-w}^{w} \varkappa_{1}^{2}(s,t) dt ds = w \int_{0}^{L} f(\varkappa, \eta, \eta') ds,$$
$$f(\varkappa, \eta, \eta') = \varkappa^{2} (1 + \eta^{2})^{2} \frac{1}{w \eta'} \log\left(\frac{1 + w \eta'}{1 - w \eta'}\right), \qquad (31)$$

where $\eta = \tau/\varkappa$. In the limit $w \to 0$, this recovers Sadowsky's functional $f(\varkappa, \eta) = 2\varkappa^2(1 + \eta^2)^2$ given in [12] where Eq. (4) for this case is obtained by applying the principle of virtual work and making use of the variation of the Frenet frame. Since the energy density f depends on derivatives of the curvature only via η , it is convenient to apply the transformation $\xi = \varkappa, \eta = \tau/\varkappa$. Equations (20) and (21) then yield $M_b = \mathcal{E}_{\varkappa}(f) - \frac{\eta}{\varkappa} \mathcal{E}_{\eta}(f), M_t = \frac{1}{\varkappa} \mathcal{E}_{\eta}(f)$. Note that $\mathcal{E}_{\varkappa}(f) = \partial_{\varkappa} f$ and hence $M_b + \eta M_t = \partial_{\varkappa} f$. These equations were first derived in [6]. The complexity of the centerline-reduced functional $f(\varkappa, \eta, \eta')$ makes this the first problem for which the invariant formulation seems to be the only way to obtain a manageable set of equilibrium equations. Their extension to intrinsically curved strips was considered in [4].

The balance equations presented here correspond to the conservation laws generated by the symmetry group of Euclidean motions [13]. A computational procedure for deriving invariant Euler-Lagrange equations [analogous to Eqs. (6) and (7)] for arbitrary finite-dimensional transformation groups can be found in [10]. When given the balance form these equations may be useful for certain problems with non-Euclidean symmetry groups. An example is the description of world lines of relativistic particles in Minkowski space with the Poincaré group of isometries as symmetry group [33,34].

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