External field influence on semiflexible macromolecules: geometric coupling

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Abstract

We suggested a geometric approach to address the external field influence on the DNA molecules, described by the WLC model via geometric coupling. It consists in the introduction of the effective metrics depending on the potential of the external field, with further re-definition of the arc-length parameter and of the extrinsic curvatures of the DNA molecules. It yields the nontrivial impact of the external field in the internal energy of macromolecules. We give the Hamiltonian formulation of this model and perform its preliminary analysis in the redefinition of the initial energy density.

1 Introduction

In recent years, single-molecule techniques have evolved into a powerful toolset for studying the dynamical behavior of many biological processes. It is now possible to follow on the nanometer and millisecond scales the individual trajectory of a single enzyme as it catalyzes a reaction, a molecular motor as it translocates, or a single polypeptide or nucleic acid molecule as it unfolds and refolds [1, 2, 3].

One of the widely used applications of single-molecule manipulations is the direct investigation of double-stranded DNA (dsDNA). The single-molecule stretching experiments gave a big contribution to the understanding of the dsDNA structure and functionality [4, 5]. The interpretation of any stretching experiment is closely related with the mechanism of elasticity. For example, the dsDNA stretching experiments are usually interpreted in terms of worm-like chains (WLC) [4, 5, 6, 7], while the ssDNA or ssRNA are usually described by freely jointed chains with elastic bonds (EFJC) [8].

The WLC Hamiltonian is presented as a functional on a differentiable space curve γ of fixed length L,

$$\mathcal{E}_0^{WLC} = \frac{l_p k_B T}{2} \int_\gamma \kappa_1^2 ds , \qquad (1.1)$$

where $\mathbf{r}(s)$ is the radius vector of an arbitrary point of the curve as a function of the contour distance s from one end to that point, T is the temperature, k_B is the Boltzmann constant, l_p is the persistence length and κ_1 is the first curvature (rigidity) of the curve, which is defined by the use of the unit vector $\mathbf{e}_1(s)$, $\mathbf{e}_1^2 = 1$ tangential to the curve: $\kappa_1 = |d\mathbf{e}_1/ds|$, $\mathbf{e}_1 = \frac{d\mathbf{r}}{ds}$, where s is the arc-length of the curve $\mathbf{r}(\tau)$,

$$s = \int_\gamma |d\mathbf{r}|, \qquad ds = |\frac{d\mathbf{r}}{d\tau}| d\tau \qquad (1.2)$$

An example of the spatial constraints, imposed on the polymer chain, is the helical structure observed in many biological and synthetic polymers [9]. In order to describe the helical structure of the chain space, following Bugle and Fujita [10] (see also [11]), we need to introduce the unit curvature vector $\mathbf{e}_2 = \frac{d\mathbf{e}_1/ds}{|d\mathbf{e}_1/ds|}$ and define the potential energy of the chain as follows:

$$\mathcal{E}_0^{BF} = \frac{k_B T}{2} \int_\gamma ds \left[(\kappa_1 - \alpha)^2 + (\kappa_2 - \beta)^2 \right], \qquad (1.3)$$

where $\kappa_1 = \dot{\mathbf{e}}_1 \cdot \mathbf{e}_2$ is a first curvature (rigidity) of γ and $\kappa_2 = \sqrt{|d\mathbf{e}_2/ds|^2 - \kappa_1^2}$ is a second curvature (torsion) of the curve γ. The α and β parameters are supposed to be the equilibrium bending and torsion constants. The absolute minimum of the potential energy is given by $\kappa_1 = \alpha$ and $\kappa_2 = \beta$ and corresponds to the regular helix with radius $r_0 = \frac{\alpha}{\alpha^2 + \beta^2}$ and pitch $h = \frac{2\pi|\beta|}{\alpha^2 + \beta^2}$.

In this respect the paper by Feoli, Nesterenko and Scarpetta [12] deserves to be mentioned. There the authors suggested to describe the DNA molecules by the functional

$$\mathcal{E}_0 = \int_\gamma (c_0 + c_1 \kappa_1) ds, \qquad (1.4)$$

whose minimum corresponds to the helical configuration of the curve. Unfortunately, these authors interpreted the functional (2.1) as a free energy of the DNA molecules, which yields some inconsistencies in the interpretation of the results. The importance of that paper is not only in the suggestion to describe the DNA molecules by the functionals linear on the curvature, but to operate with the functionals depending on extrinsic curvatures by the use of the Dirac's theory of constrained systems [13]. Further below, we will discuss this issue in more detail.

It is not occasional, that in all listed models the energy of the macromolecule is defined by the use of extrinsic curvatures of the macromolecule curve. Indeed, the (linear) density of the energy of the macromolecule should *a priori* depend on the geometric characteristic of the curves and be independent on the way of their description. Hence, it should depend on the functions of the curve γ which are invariant under its motions (rotations and translations), i.e. on its extrinsic curvatures κ_I, $0 < I \leq D - 1$ (where D is the dimensionality of the space) [14]

From this viewpoint the common approach, for taking into account the external field influence, seems to be ill-defined. It consists in the naive adding to the energy functional given further below in (2.1) of the potential energy term [15]

$$\mathcal{E} = \mathcal{E}_0 + \int_\gamma V(\mathbf{r}) ds, \tag{1.5}$$

where $V(\mathbf{r(s)})$ is the potential of the external field.

The geometric ("macroscopic") inconsistency is that the energy functional of the macromolecule becomes the function of a quantity, which is not invariant under the motions of the curve (rotations and translation in Euclidean space).

The physical ("microscopic") inconsistency of this approach is the independence of the chain flexibility (e.g. the persistence length l_p) on the external field. While the stretching or the compressing fields substantially restricted the set of available conformations of each repeated unit of the polymeric chain. Thus, a strong enough external field should affect the chain flexibility, and the persistence length l_p. This issue should be relevant, e.g. for the confinement-induced changes of the persistence length observed in [16]. The effective compressing field, describing the intra - chain attraction and chain confinement in restricted geometries yields a substantial change of the apparent persistence length [17, 18].

The purpose of the present paper is to suggest an alternative way for taking into account the external field influence, which seems to be free from the above discrepancies. Namely, we suggest to involve the external field in the definition of the line element ds, associating it with the effective metric

$$g_{AB} = (1 + V(\mathbf{r}))^2 \delta_{AB} \equiv n^2(\mathbf{r}) \delta_{AB}, \tag{1.6}$$

and to define the extrinsic curvatures κ_I, in accordance with Frenet equations, on the space equipped with this effective metric.

Hence, we suggest to preserve the functional dependence of the energy density from the extrinsic curvature, but modify the definition of the arc-length, and consequently, of the extrinsic curvatures.

The paper is organized as follows.

In the Second section we present the explicit expression of the suggested geometric model of the macromolecule interaction with the external field, and discuss the analogies of this model with relativistic particle systems and with geometric optics.

In the Third section we give its Hamiltonian formulation and analyze it in the framework of the Dirac's theory of constrained systems.

2 The model

We suggest to describe the external field influence on the macromolecule by the energy functional

$$\mathcal{E}_0 = \int_\gamma F(\kappa_1, ..., \kappa_N) d\widetilde{s}, \tag{2.1}$$

where

- $F(\kappa_I)$ is the energy density in the initial (noninteracting) DNA model. It can be chosen say, as in (1.1), (1.3), (1.4)

- The element of arclength (or control length) $d\widetilde{s}$ is defined in accordance with the metric (1.6),

$$d\widetilde{s} = n(\mathbf{r})|\dot{\mathbf{r}}|d\tau \equiv \dot{\widetilde{s}}d\tau, \tag{2.2}$$

where τ is an arbitrary parameter defining the curve γ: $\mathbf{r} = \mathbf{r}(\tau)$

- The extrinsic curvatures κ_I are defined, via Frenet equations, on the space equipped by the effective metric (1.6),

$$\frac{d\mathbf{r}}{\dot{s}d\tau} = \mathbf{e}_1, \qquad \frac{D\mathbf{e}_a}{\dot{s}d\tau} = \kappa_a \mathbf{e}_{a+1} - \kappa_{a-1}\mathbf{e}_{a-1}. \tag{2.3}$$

Here

$$\frac{D}{d\tau} \equiv \frac{d}{d\tau} + \widehat{\Gamma}(\dot{\mathbf{r}}), \quad (\widehat{\Gamma})^A_B \equiv \Gamma^A_{BC}\dot{x}^C, \qquad \mathbf{e}_a \cdot \mathbf{e}_b = \delta_{ab}, \quad \mathbf{e}_0 = \mathbf{e}_{D+1} \equiv 0, \ I = 1, \ldots, D$$

with $\mathbf{e}_i\mathbf{e}_j \equiv e^{(i)A}g_{AB}e^{(j)B}$, being D the dimensionality of the space and Γ^A_{BC} the Christoffel symbols of the effective metric

$$\Gamma^C_{AB} = n_A\delta_{CB} + n_B\delta_{CA} - n_C\delta_{AB}, \qquad n_A \equiv \partial_A \log n. \tag{2.4}$$

Similarly to the Euclidean case, the curvatures $\kappa_1, \ldots, \kappa_{D-1}$ are positive functions, and the highest curvature (torsion), κ_{D-1} can take both positive and negative values. If some $\kappa_I \neq 0$, then $\kappa_i \neq 0$ $i = 1, 2, \ldots, I-1$. Vice versa, from $\kappa_I = 0$, it follows that $\kappa_i = 0$ $\mu = I+1, \ldots, D-1$.

Explicit expressions for external curvatures look as follows:

$$\kappa_I = \frac{\sqrt{\det \hat{g}_{I+1} \det \hat{g}_{I-1}}}{\det \hat{g}_I}, \qquad (g_I)_{ij} \equiv \frac{d^i\mathbf{r}}{(d\widetilde{s})^i}\frac{d^j\mathbf{r}}{(d\widetilde{s})^j}, \quad i, j = 1, \ldots, I. \tag{2.5}$$

In particular, the first curvature κ_1 reads

$$\kappa_1 = \frac{1}{n^2(\mathbf{r})}\sqrt{\kappa^2_{(flat)1} + \frac{\dot{n}^2}{|\dot{\mathbf{r}}|^2 n^4}}, \tag{2.6}$$

where $\kappa_{(flat)1}$ is the first curvature of the curve on the flat space. Hence, within the suggested approach, we have got the geometrically consistent energy functional of the macromolecule, where the influence of the external field in the internal energy is taken into account. Since we deal with the macroscopic model (or a phenomenological description) of the macromolecule, we can assume that $n(\mathbf{r})$ parametrically depends on the temperature T. For the correspondence with the existing models we can choose, e.g. $n = n(T, \mathbf{r}) = k_B T(1 + \frac{V(\mathbf{r})}{k_B T})$. The environment influence on the chain elasticity and flexibility is usually described in terms of the persistence length. For example, to describe the DNA behavior in nanochannels and nanoslits, the concept of the global persistence length has been introduced in [19], as a typical distance between hairpins in the confined chain. The main advantage of the obtained result is the deep non-trivial relationship between the bending elasticity and the external field. The proposed approach seems to be useful for a better understanding of the mechanism of elasticity of macromolecules, in stretching and confining fields.

The price for the geometrization of the model is the further mathematical complication of the system. In spite of the apparent simplicity, the analysis of models with the energy functional (2.1) is not a simple task: the matter is that the energy density F in (2.1) depends on higher derivatives and should be analyzed in the framework of the Dirac's theory of constrained systems [13]. Fortunately, in the eighties such functionals were widely studied in the context of the (relativistic) spinning particles. Namely, the functionals (2.1) in the Minkowski space-time, with s being a world-line parameter were considered. These studies were inspired by the papers Polyakov devoted to the Chern-Simons theories and rigid strings [20]. Various systems depending on the first and the second curvatures of the path in three- and four- dimensional Minkowski spaces were studied in details, mostly by Plyushchay (see [21, 22] and references therein). By this reason the relevant formalism for analyzing such systems on the base of the Frenet equations has been developed by one of the authors [23]. Almost all systems depending on extrinsic curvatures either by isospin (i.e. by internal degrees of freedom), or spin (in the case when they are proportional to a single curvature, see [22, 24]. In the context of macromolecules it means, that the systems with energy density depending on extrinsic curvatures of macromolecules should have internal degrees of freedom. Now, any macromolecule is a sequence of atoms connected by chemical bonds. That is why, the

universal way of any change of chain conformation is the change of dihedral angles, caused by rotation around the chemical bonds. Thus, any polymeric chain has its internal rotational degrees of freedom, which should be obviously identified with the isospin of the system. These studies were performed on flat spaces, mostly. The only exceptions are, seemingly [25, 24]. A qualitative observation there is that, for Lagrangians (in our case: energy densities) with linear dependence on extrinsic curvatures, the introduction of non-Euclidean metrics drastically changes the properties of the system, including the dimensionality of the internal space. Only for the constant curvature spaces (e.g. spheres, hyperboloids) non-Euclidean metrics do not change essentially the properties of such systems. In three-dimensional space, in our notation it corresponds to the choice

$$n(\mathbf{r}) = \alpha_0/(1 + \beta\mathbf{r}^2) \tag{2.7}$$

corresponding to the three-dimensional sphere or hyperboloid (depending on the choice of the sign of β).

The suggested DNA model has an obvious analogy with the geometric optic, where the trajectory of light in the media with refraction index $n(\mathbf{r})$ corresponds to the minimum of the functional (under assumption that the helicity of light is neglected)

$$\mathcal{S}_{Fermat} = \int d\widetilde{s}, \qquad d\widetilde{s} = n(\mathbf{r})|\dot{\mathbf{r}}|d\tau. \tag{2.8}$$

Hence, the generic action (2.1) defined on such "effectively" curved space, will take into account the interaction of the spin (helicity) of the light with the media, i.e. the phenomenon of the "optical Hall effect", consisting in the deviation of the light trajectory from that given by Fermat Principle, due to the feedback from the polarization [26]. Let us also mention, in this respect, the recent paper [27], where the analysis of the model (1.4) with a non-constant effective metric has been performed in some details, in the context of geometric optic.

So, we suggest to describe the DNA molecules interacting with the external field by the functional (2.1), where the arc-length is defined by the expression $d\widetilde{s} \equiv (1 + V(\mathbf{r}))|\dot{\mathbf{r}}|d\tau$, and the extrinsic curvatures $\kappa_1, \ldots, \kappa_N, N < D$ are defined in accordance with modified Frenet equations (2.3).

3   Hamiltonian formulation

It is seen from the Frenet equations (2.3), that the I-th extrinsic curvature κ_I depends on the $(I+1)$-th derivative, $\kappa_I = \kappa_I(\mathbf{r}^{(i)})$, so that the energy density $F(\kappa_i)$ in (2.1) depends on the $(N+1)$-th derivative. By this reason the study of its Euler-Lagrange equations is not a simple task. To simplify the analysis of (2.1), let us consider the variationally equivalent functional, whose integrand depends on the first derivatives only (see [23, 24, 28] for further details).

Precisely, we replace the initial energy density $\mathcal{L}$ by the following variationally equivalent one:

$$\widetilde{F} = F(\kappa_1, \ldots, \kappa_N) - \lambda \left(\kappa_N - \sqrt{\left(\frac{D\mathbf{e}_N}{\dot{\widetilde{s}}d\tau}\right)^2 - \kappa_{N-1}^2} \right)$$

$$+ \mathbf{p}\left(\frac{d\mathbf{x}}{\dot{\widetilde{s}}d\tau} - \mathbf{e}_1\right) + \sum_{i-1} \mathbf{p}_{i-1}\left(\frac{D\mathbf{e}_{i-1}}{\dot{\widetilde{s}}d\tau} - \kappa_{i-1}\mathbf{e}_i + \kappa_{i-2}\mathbf{e}_{i-2}\right) - \sum_{i,j} d^{ij}\left(\mathbf{e}_i\mathbf{e}_j - \delta_{ij}\right), \tag{3.1}$$

where $\dot{\widetilde{s}}, \kappa_{i-1}, d^{ij}, \mathbf{p}_{i-1}, \mathbf{e}_i, \lambda$ play the role of independent variables, and the relation

$$\kappa_N^2 = \left(\frac{D\mathbf{e}_N}{\dot{s}d\tau}\right)^2 - \kappa_{N-1}^2,$$

which follows from (2.3) is taken into account. Here and further below, we use the following notation for the scalar products: $\mathbf{p}_i \cdot \mathbf{p}_j \equiv p_{(i)A}g^{AB}p_{(j)B}$, $\mathbf{p}_i \cdot \mathbf{e}_j \equiv p_{(i)A}e_j^A$, where, upon summation the indices A, B take the values $1, \ldots, D$, and $i, j = 1, \ldots, N$.

It is easy to see, that varying the energy density $\widetilde{F}$ by κ_N, we shall get $\lambda = \partial F/\partial\kappa_N$, while its variations by $\mathbf{p}, \mathbf{p}_{i-1}$ and d_{ij} will yield the Frenet equations restoring the dependence of κ_i on $\mathbf{r}^{(i)}$.

The Hamiltonian formulation of the system with the singular "Lagrangian" (3.1) on the Euclidean space was carried out in [23]. Its extension to curved space is straightforward. For the "Lagrangians" linear on extrinsic

curvatures it was considered in [24], and for the generic case in [28]. In accordance with this paper, the Euler-Lagrange equations of the functional with the energy density $\widetilde{F}$ are given by the constrained Hamiltonian system,

$$\omega_N = d\mathbf{p} \wedge d\mathbf{r} + \sum_{i=1}^{N} d\mathbf{p}_i \wedge d\mathbf{e}_i, \qquad H = h_0 + \sum_i \kappa_i \phi_i + \sum_{i,j} d^{ij}(\mathbf{e}_i \mathbf{e}_j - \delta_{ij}), \tag{3.2}$$

with the following set of constraints (including some gauge fixing conditions, see for details [23, 28]):

$$\phi_0 \equiv \boldsymbol{\pi} \mathbf{e}_1 + \sum_i \kappa_i F_{,i} - F \approx 0, \qquad \text{where } \boldsymbol{\pi} \equiv \mathbf{p} - \boldsymbol{\Gamma}, \quad \Gamma_A \equiv \sum_{i=1}^{N} \Gamma_{AB}^{C} p_{(i)C} e_i^{B} \tag{3.3}$$

$$\mathbf{p}_i \mathbf{e}_j \approx 0, \quad i \geq j \tag{3.4}$$

$$\mathbf{e}_i \mathbf{e}_j - \delta_{ij} \approx 0, \tag{3.5}$$

$$\phi_{i-1} \equiv \mathbf{p}_{i-1}\mathbf{e}_i - \mathbf{p}_i \mathbf{e}_{i-1} - F_{,i-1} \approx 0, \quad 2\phi_N = \frac{1}{F_{,N}}\left(\mathbf{p}_N\mathbf{p}_N - \sum_i (\mathbf{p}_N\mathbf{e}_i)(\mathbf{p}_N\mathbf{e}_i)\right) - F_{,N} \approx 0 \tag{3.6}$$

For $\det \partial^2 F/\partial\kappa_i \partial\kappa_j \neq 0$, we can resolve the equations (3.6), expressing κ_i via $\mathbf{p}_i, \mathbf{e}_j$. After that we should substitute these expressions for κ_i in (3.3).

Otherwise, for $corank\ \partial^2 F/\partial\kappa_i\partial\kappa_j = M \neq 0$, we can resolve only $(N - M)$ equations in (3.6), while the rest will appear as a primary constraint, with the M undefined functions on κ_i playing the role of Lagrangian multipliers.

After these manipulations we will get the constrained Hamiltonian system with $N(N-1)+1$ primary constraints given by (3.3)-(3.5) and with M primary constraints obtained from (3.6). Then, we should perform the Dirac's procedure of "stabilization" of the above set of constraints, i.e. require $\{\ldots, H\} \approx 0$, where by $\ldots$ we encoded the set of primary constraints. This requirement will either fix the values of Lagrangian multipliers, or yield an additional set of "secondary" constraints. Then, stabilizing the obtained set of secondary constraints, we shall either get the new set of secondary constraints, or will further fix the values of Lagrangian multipliers, and so on (see, e.g., [13]).

It is easy to observe, that the "stabilization" of the constraints (3.4) fixes the values of the Lagrangian multipliers d^{ij}, while the stabilization of the remaining set depends on the concrete properties of the function $F(\kappa_1, \ldots, \kappa_N)$.

For example, for the energy densities with a non-degenerate quadratic dependence on curvatures, $F = c_{ij}\kappa_i\kappa_j$, $\det c_{ij} \neq 0$, which involves, as a particular case, the WLC model (1.1) and Buggle-Fujita model (1.3), there are no secondary constraints. The whole set of (primary) constraints is divided in the second-class constraints given by (3.4),(3.5), and the single first-class constraint given by (3.3). As a consequence, we get that the dimensionality of the physical phase space is $2D(N + 1) - 2 - N(N - 1) = 2DN - N(N - 1)$. In contrast with this case, in the systems with linear energy densities, $F = c_i\kappa_i + c_0$, the whole set of constraints and their algebra, essentially depend on the values of the constants c_i and on the properties of the effective metric (1.6).

Hence, in contrast with the functionals with linear dependence on curvature, in the case of quadratic dependence, the introduction of the curved metric does not essentially change the structure of the phase space of the system, being reflected only on the functional dependence of the Hamiltonian from the external field.

To complete this general consideration, let us present the following useful expressions, which should be useful for the further analysis of the systems under consideration.

At first, let us write down the non-zero Poisson brackets between the functions $\boldsymbol{\pi}e_i$, $\boldsymbol{\pi}\mathbf{p}_i$, $\boldsymbol{\pi}^2$:

$$\begin{aligned}
\{\boldsymbol{\pi}\mathbf{e}_i, \boldsymbol{\pi}\mathbf{e}_j\} &= \mathcal{R}(\mathbf{e}_i, \mathbf{e}_j), \quad \{\boldsymbol{\pi}\mathbf{p}_i, \boldsymbol{\pi}\mathbf{p}_j\} = \mathcal{R}(\mathbf{p}_i, \mathbf{p}_j) \\
\{\boldsymbol{\pi}\mathbf{e}_i, \boldsymbol{\pi}\mathbf{p}_j\} &= \mathcal{R}(\mathbf{e}_i, \mathbf{p}_j) - \boldsymbol{\pi}^2\delta_{ij}, \quad \{\boldsymbol{\pi}\mathbf{e}_i, \boldsymbol{\pi}^2\} = -2\mathcal{R}(\boldsymbol{\pi}, \mathbf{e}_i), \quad \{\boldsymbol{\pi}\mathbf{p}_i, \boldsymbol{\pi}^2\} = -2\mathcal{R}(\boldsymbol{\pi}, \mathbf{p}_i)
\end{aligned} \tag{3.7}$$

where

$$\mathcal{R}(\mathbf{a}, \mathbf{b}) \equiv \sum_{i=1}^{N} R(\mathbf{p}_i|\mathbf{e}_i, \mathbf{a}, \mathbf{b}). \tag{3.8}$$

is the Riemann tensor associated with the effective metric (1.6).

Then, let us present the expression for the Riemann tensor in the three-dimensional space, where it is uniquely expressed via the Ricci tensor

$$R_{ABCD} = R_{(2)AC}g_{BD} - R_{(2)AD}g_{BC} + R_{(2)BD}g_{AC} - R_{(2)BC}g_{AD} + \frac{R_0}{2}\left(g_{AD}g_{BC} - g_{AC}g_{BD}\right), \tag{3.9}$$

where R_2 is the Ricci tensor and R_0 is the scalar curvature of the space. For the conformal flat metric (1.6) the Ricci tensor is defined by the formulae

$$R_{AC} = -g_{AC}(n_{DD} + 3n_D^2) - n_{A,C} + n_A n_C, \qquad n_A \equiv \partial_A \log n. \tag{3.10}$$

All considerations above were quite general, with a generic functional dependence of the energy density on the extrinsic curvatures, and they have been formulated in the D-dimensional space. As an example, let us give the explicit formulation of the WLC model (1.1), with the additional constant term c_0

$$F = \frac{c}{2}\kappa_1^2 + c_0. \tag{3.11}$$

In this case the Hamiltonian system (3.2) reads

$$\omega = d\mathbf{p} \wedge d\mathbf{r} + d\mathbf{p}_1 \wedge d\mathbf{e}_1, \qquad H = \boldsymbol{\pi}\mathbf{e}_1 + \frac{\mathbf{p}_1^2}{2c} - c_0 + \left(c_0 - \frac{3}{2}\boldsymbol{\pi}\mathbf{e}_1\right)(\mathbf{e}_1 \cdot \mathbf{e}_1 - 1), \tag{3.12}$$

with the following set of constraints:

$$\mathbf{e}_1 \cdot \mathbf{e}_1 - 1 \approx 0, \quad \mathbf{p}_1 \cdot \mathbf{e}_1 \approx 0, \quad \boldsymbol{\pi}\mathbf{e}_1 + \frac{\mathbf{p}_1^2}{2c} - c_0 \approx 0. \tag{3.13}$$

The extrinsic curvatures looks as follows:

$$\kappa_1 = \sqrt{\frac{\mathbf{p}_1^2}{c^2}}, \qquad \kappa_2^2 = \frac{1}{c^2\kappa_1^2}\left(\boldsymbol{\pi}^2 - 4c_0\boldsymbol{\pi}\mathbf{e}_1 + \frac{3}{4}(\boldsymbol{\pi}\mathbf{e}_1)^2 + c_0^2\right) - \kappa_1^2. \tag{3.14}$$

The evolution equations for these curvatures could be straightforwardly obtained by the use of Poisson bracket relations (3.7). They will obviously depend from the Riemann tensor (3.8).

We suppose to present the detailed study of the WLC model in a forthcoming paper.

4   Conclusion

In this paper we suggested a geometric approach to address the external field influence on the DNA molecules, described by the WLC model via geometric coupling. It consists in the introduction of the effective metrics depending on the potential of the external field, with further re-definition of the arc-length parameter and of the extrinsic curvatures of the chain. It yields a nontrivial impact of the external field in the internal energy of macromolecules, and the natural changes of the persistent length. We gave the Hamiltonian formulation of this model and performed its preliminary analysis in terms of Dirac's theory of constrained systems. Particularly, we have shown, that such coupling does not change the number of internal degrees of freedom in the models with quadratic dependence on extrinsic curvatures. The parallels of the presented DNA model with spinning particles on curved space, as well as with geometric optics, allows us easily to evaluate qualitative properties of the systems, as well as to involve, in the study of the DNA macromolecules, the tools of symplectic and Riemann geometry, and of the relativistic quantum mechanics.

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