MODELING THE INTERACTIONS OF BIOMATTER AND BIOFLUID

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The internal motions of biomatter immersed in biofluid are investigated. The interactions
between the fragments of biomatter and its surrounding biofluid are modeled using field
theory. In the model, the biomatter is coupled to the gauge field representing the biofluid.
It is shown that at non-relativistic limit various equation of motions, from the well-known
Sine-Gordon equation to the simultaneous nonlinear equations, can be reproduced within
a single framework.

Keywords: biomatter; biofluid; soliton.

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1. Introduction

The deoxyribonucleic acid (DNA) is getting the very important biomolecules. Es-
pecially its helical structures undergoes a very complex dynamics and plays several
important roles in various biological phenomena such as storage of information, in-
heritance (replication, etc) and the usage of genetic information (transcription, etc).
Physically, transcription processes begin with the open state in the DNA double he-
lix. The phenomena describe the internal DNA mobility such as rotational motion
of nitrous bases, asymmetry of the helix, strength of the hydrogen bond and so on
1 The rotational motion mode with such asymmetry has a solitary wave solution
describing the open state of double helix2.

DNA is not motionless. It is in a constantly wriggling dynamics state in a
medium of bio-organic fluid in the nucleus cell. One can think of the DNA molecule
as behaving somewhat like a microscopic piece of worm-like elastic suspended in
solution. In this approximation, one ignores all details of the chemical structure. The motion of DNA surrounded by fluid is rarely studied. Previous studies are usually done by solving the fluid equations and its wave equations simultaneously using appropriate boundary conditions. For example, the thermal denaturation of double strand DNA depends on the solution surrounding the DNA molecules. It is necessary to take into consideration that the solving water does act as a viscous medium and may damp out bubble denaturation. The impact of viscosity has been investigated by Zdrakovic et al. which shows that the behavior of DNA dynamics in viscous solution is described by the damped nonlinear Schrödinger (NLS) equation. The solution is then obtained by expansion and performing order-by-order calculation. In these approaches, anyway the picture of interaction between DNA and its surrounding fluid is not clear. Also, in most models the over-damped DNA dynamics are treated by putting some additional terms by hand in the differential equation to obtain the non-homogeneous ones.

There is a technology for DNA manipulation developed in the last decade using gel electrophoresis. This technique is used to estimate the size of genetic sequences and understand the dynamics of individual strands of DNA as they move through a fluid solution. In theoretical polymer dynamics, the study is mostly focused on describing single-polymer dynamics to improve models of bulk properties. All of them attempt to understand the behavior of individual polymers under controlled fluid flows through the Navier-Stokes equation coupled with elastic strings. Theoretical studies of this matter is still an open problem, especially related to rheological problem.

In this paper, we study the soliton excitation in DNA with surrounding fluid based on the gauge field theory formulation. The DNA dynamics is modeled as the result of interactions among matters in a fluid medium using the relativistic and gauge invariant fluid dynamics lagrangian. The theory is a relativistic one, but we can take its non-relativistic limit at the final stage to deal with problems in biomatter as done in some previous works, like in some models using the ideal gas approximation, Sine-Gordon models etc. The lagrangian is originally devoted to model the magnetofluid in plasma as a relativistic fluid system inspired by the similarity between the dynamical properties of fluid and electromagnetic field. Within the model, the interactions of DNA and fluid dynamics are described in a general way as the results of interactions among the fluid and matter fields.

The paper is organized as follows. In the first chapter the model of interaction between biomolecule and fluid is given. It is then applied to describe the dynamics of worm-like DNA molecule with varying velocity. The paper is finally ended by a summary.

2. The model

Some mechanical models of DNA have been proposed over the years which are focused on different biological, physical and chemical processes in which DNA is
involved. One of the important model related to the identification of the unwinding of double helix in a "bubble" is called the torsional $Y$ model. The lagrangian describing the bubble of $Y$ model is represent by a scalar (boson) field governed by the bosonic lagrangian:

$$L_{\text{matter}} = (\partial_{\mu} \Phi)^\dagger (\partial^\mu \Phi) + V(\Phi),$$  \quad (1)

where $V(\Phi)$ is the potential. For example in the typical $\Phi^4$—theory,

$$V(\Phi) = \frac{1}{2} m^2 \Phi \Phi^\dagger - \frac{1}{4!} \lambda (\Phi^\dagger \Phi)^2,$$  \quad (2)

where $m_\Phi$ and $\lambda$ are the mass of matter and the nonlinear constant. The hermite conjugate is $\Phi^\dagger \equiv (\Phi^\ast)^T$ for a general complex field $\Phi$ describing a rotational (torsional motion) of DNA.

The interaction in the $Y$ model with fluid medium is described in the gauge field theory framework. In this theory, the above bosonic lagrangian is imposed to be gauge invariant under local (in general non-Abelian) gauge transformation, $U \equiv \exp[\frac{1}{i} T^a(\theta^a(x))] \approx 1 - \frac{1}{2} T^a(\theta^a(x))$ with $\theta^a \ll 1$. $T^a$'s are generators belong to a particular Lie group and satisfy certain commutation relation $[T^a, T^b] = i f^{abc} T^c$ with $f^{abc}$ is the anti-symmetric structure constant. The matter field is then transformed as $\Phi U^{-1} \to \Phi' \equiv \exp[\frac{1}{i} T^a(\theta^a(x))] \Phi$, with $T^a$ are $n \times n$ matrices while $\Phi$ is an $n \times 1$ multiplet containing $n$ elements. It is well-known that the symmetry in Eq. (1) is revealed by introducing gauge fields $A^a_{\mu}$ which are transformed as $U^a_{\mu} \to U'^a_{\mu} \equiv U^a_{\mu} - \frac{1}{2} (\partial_{\mu} \theta^a) + f^{abc} \theta^b U^c_{\mu}$, and replacing the derivative with the covariant one, $D_{\mu} \equiv \partial_{\mu} + ig T^a U^a_{\mu}$. The fluids is represent by the gauge fields that guarantees the invariant properties of the system. Then the total lagrangian with some additional terms to keep its gauge invariance is,

$$\mathcal{L} = \mathcal{L}_{\text{matter}} + \mathcal{L}_{\text{gauge}} + \mathcal{L}_{\text{int}},$$  \quad (3)

where,

$$\mathcal{L}_{\text{gauge}} = -\frac{1}{4} S^a_{\mu\nu} S^{a\mu\nu},$$  \quad (4)

$$\mathcal{L}_{\text{int}} = -g J^a_{\mu} U^a_{\mu} + g^2 (\Phi^\dagger T^a T^b \Phi) U^a_{\mu} U^b_{\mu}.$$  \quad (5)

The strength tensor is $S^a_{\mu\nu} \equiv \partial_{\mu} U^a_{\nu} - \partial_{\nu} U^a_{\mu} + g f^{abc} U^b_{\mu} U^c_{\nu}$, while the 4-vector current is,

$$J^a_{\mu} = -i \left[ (\partial_{\mu} \Phi)^\dagger T^a \Phi - \Phi^\dagger T^a (\partial_{\mu} \Phi) \right].$$  \quad (6)

The coupling constant $g$ then represents the interaction strength between gauge field and matter. We should note that, however the current conservation is realized by the covariant current $\partial_{\mu} J^a_{\mu} = 0$ with $J^a_{\mu} \equiv -i \left[ (\partial_{\mu} \Phi)^\dagger T^a \Phi - \Phi^\dagger T^a (\partial_{\mu} \Phi) \right]$.

The gauge boson $U_{\mu}$ is interpreted as a "fluid field" with velocity $u_{\mu}$, and takes the form:

$$U^a_{\mu} = (U^0_{\mu}, U^a) \equiv u^a_{\mu} \phi,$$  \quad (7)
with,
\[ u_\mu^a = \gamma^a (1, -v^a) , \]  
(8)

where \( \phi \) is an auxiliary boson field, while \( \gamma^a \equiv (1 - |v^a|^2)^{-1/2} \). Here we adopt the natural unit, i.e. the light speed \( c = 1 \). We should remark that the auxiliary field \( \phi \) is introduced to keep correct dimension.

For microfluid one usually works with a single fluid. From the gauge theory point of view, this is realized by the Abelian gauge lagrangian. The total lagrangian in this case becomes,
\[ L = \left( \partial_\mu \Phi^* \right) \left( \partial^\mu \Phi \right) + \frac{1}{2} m_\Phi^2 \Phi^* \Phi - \frac{1}{4!} \lambda (\Phi^* \Phi)^2 + g^2 U_\mu U^\mu \Phi^* \Phi \]
\[ - \frac{1}{4} (\partial_\mu U_\nu - \partial_\nu U_\mu) (\partial^\mu U^\nu - \partial^\nu U^\mu) + ig U^\mu \left[ (\partial_\mu \Phi^*) \Phi - \Phi^* (\partial_\mu \Phi) \right] , \]
(9)

using Eqs. (2), (3) \( \sim (5) \) and (6). The strength tensor is given by \( S_{\mu \nu}^a \equiv \partial_\mu U_\nu^a - \partial_\nu U_\mu^a \).

The non-relativistic limit can be obtained by performing a transformation \( t \rightarrow \tau \equiv it \) and putting \( \gamma \rightarrow 1 \) respectively. Imposing the variational principle of action, one reaches at the Euler-Lagrange equation \( \Phi \). Therefore, the equation of motion (EOM) for \( \Phi \) reads,
\[ \left( \partial^2 - m_\Phi^2 - 2g^2 |v|^2 \right) \Phi + \frac{1}{3!} \lambda \Phi^3 = 0 . \]
(10)

for a real \( \Phi \) field. This result leads to the well-known nonlinear Klein-Gordon equation. On the other hand, the EOM of \( U_\mu \) is given by,
\[ \frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{v} = -g \mathbf{F} , \]
(11)

where \( \mathbf{v} \) is fluid velocity in non-relativistic limit. \( \mathbf{F} \) is total external force (see [7] for detail derivation). This is the model the underlying model throughout this paper.

3. DNA dynamics in the surrounding fluid

Behavior of the DNA interaction with surrounding fluid depends on the boundary condition of fluid phenomena. One should deal with the boundary value problem for the fluid equation and then solve the DNA dynamics through Eq. (10). For the sake of simplicity, however let us fix the fluid flow in order to avoid solving the boundary value problem.

3.1. Constant Velocity

First of all, consider \( \mathbf{v} = \mathbf{v}_0 \) is a constant and write down Eq. (10) in the standard form,
\[ \frac{\partial^2 \Phi}{\partial t^2} - \frac{\partial^2 \Phi}{\partial x^2} - \tilde{m}_\Phi^2 \Phi + \lambda \Phi^3 = 0 , \]
(12)
in term of coordinate \((t, x)\), where \(\bar{m}_\Phi^2 \equiv m_\Phi^2 + 2g^2v_0^2\). It’s well known that the solution of the equation can be represented by the Jacobi elliptic function \(^9\).

For \(\lambda > 0\) the solution is,

\[
\Phi(x, t) = A\bar{m}_\Phi \text{sn} \left[ \beta(x + x_0 - Ct), m \right],
\]

where \(\beta = \sqrt{\lambda \bar{m}_\Phi^2 / ((1 - C^2)(1 + m))}\), \(A = \sqrt{2m/(1 + m)}\), \(C\) is the phase velocity and \(m\) is a modulus. In the limit \(m \to 1\), one obtains the usual kink solitary waves as follow,

\[
\Phi(x, t) = \bar{m}_\Phi \text{tanh} \left[ \sqrt{\frac{\lambda \bar{m}_\Phi^2}{2(1 - C^2)}}(x + x_0 - Ct) \right].
\]

For \(\lambda < 0\) the solution is,

\[
\Phi(x, t) = A\bar{m}_\Phi \text{dn} \left[ \beta(x + x_0 - Ct), m \right],
\]

where \(\beta = \sqrt{-\lambda \bar{m}_\Phi^2 / ((1 - C^2)(2 - m))}\) and \(A = \sqrt{2/(2 - m)}\). In the limit of \(m \to 1\), one obtains the pulse solitary wave solution,

\[
\Phi(x, t) = \bar{m}_\Phi \sqrt{2 \text{sech}} \left[ \sqrt{\frac{-\lambda \bar{m}_\Phi^2}{1 - C^2}}(x + x_0 - Ct) \right].
\]

Therefore, one has two kind of solutions, namely the kink solution and the pulse solitary wave solution. These solutions can be usually used to describe the propagation of a bubble in a torsional motion of the \(Y\) model.

3.2. Velocity as a small perturbation

In this subsection, let us assume that the DNA-fluid interactions lead to small perturbation of the homogeneous solution. In this case a linear perturbation technique can be used. One can rewrite the EOM as follow,

\[
\frac{\partial^2 \Phi}{\partial t^2} - \frac{\partial^2 \Phi}{\partial x^2} \Phi + \lambda \Phi^3 = 0,
\]

According to the linear perturbation theory, the solution of Eq. \((17)\) can be treated perturbatively,

\[
\Phi(x, t) = \Phi_0(x, t) + \epsilon \Phi_1(x, t),
\]

where \(\epsilon\) is a small parameter, i.e. \(v^2(x, t) \sim \epsilon\). Substituting Eq. \((18)\) into Eq. \((17)\) leads to the following equation,

\[
\frac{\partial^2 \Phi_0}{\partial t^2} - \frac{\partial^2 \Phi_0}{\partial x^2} \Phi_0 + \lambda \Phi_0^3 = 0,
\]

for the zeroth order and,

\[
\frac{\partial^2 \Phi_1}{\partial t^2} - \frac{\partial^2 \Phi_1}{\partial x^2} + V^2(x, t) \Phi_1 = 0,
\]

where \(V \equiv \sqrt{2} \text{sn} \left[ \beta(x + x_0 - Ct), m \right]\).
for the first order. Here $V^2(x, t) = (-m^2_0 - 2g^2v^2(x, t) + 3\lambda\Phi_0^2)$. Eq. (19) is an ordinary nonlinear Klein-Gordon equation, while Eq. (20) is the linear Klein-Gordon equation with coefficient variable.

$\Phi_0$ is a solution of Eq. (19) which is the term of Jacobi elliptic functions (Eqs. (13) ~ (16)). The solution is the function of variable $x' = x - Ct$. To solve Eq. (20) and by assuming that $v(x, t) = v(x')$, one needs to introduce new variables, $x' = x - Ct$ and $t' = t - Cx$. In the new coordinate, Eq. (20) reads,

$$\frac{\partial^2 \Phi_1}{\partial t'^2} - \frac{\partial^2 \Phi_1}{\partial x'^2} + V^2(x')\Phi_1 = 0 ,$$

(21)

This result yields that the solution has the form of,

$$\Phi(x', t') = \phi(x')e^{-i\omega t'} .$$

(22)

Then substituting this result into Eq. (21), one immediately gets the Sturm-Liouville equation,

$$-\frac{d^2 \phi}{dx'^2} + \tilde{V}^2(x')\phi = 0 ,$$

(23)

where $\tilde{V}^2(x') = V^2(x) - \omega^2$. In principles using the WKBJ expansion technique, the solution of this equation can be obtained. One should notice that the solution is exist only when the 'potential' slowly varies with $x'$.

First, write $\tilde{V}(\epsilon x') = \tilde{V}(X)$ with $X$ is the scale and $\epsilon \ll 1$. One has,

$$-\epsilon^2 \frac{d^2 \phi}{dX^2} + \tilde{V}(X)\phi = 0 ,$$

(24)

and the solution is [10],

$$\phi(X, \epsilon) = \frac{C_0}{\sqrt{\tilde{V}(X)}}\exp \left[ -\frac{i}{\epsilon} \int^{x'} \tilde{V}(\xi)d\xi \right] + \frac{C_1}{\sqrt{\tilde{V}(X)}}\exp \left[ \frac{i}{\epsilon} \int^{x'} \tilde{V}(\xi)d\xi \right] + O(\epsilon) .$$

(25)

One can also study another case with fluid velocity having the form of $U(x) = \sin(x)$.

### 3.3. Stratified velocity

One of the important experiments is the DNA (biopolymer) dynamics in shear flow [5]. The experiment shows that in a steady shear flow, the molecules continually fluctuate between nearly fully coiled and fully stretched conformation while undergoing end-over-end tumbling. The fluctuations between conformations are aperiodic and exhibited a power law roll-off at a high frequency, which is attributed to a tumbling instability driven by Brownian motion.

In the model, the calculation of shear effect on the dynamics within the Y model is easy to describe. The description of such DNA bubble dynamics in shear flow is geometrically depicted in Fig. [4].
In the microfluid experiments, the fluid is usually treated one dimensionally and assumed to be incompressible, non-inertia, fully developed, unidirectional, Newtonian and steady flow. Under these assumptions, the EOM for fluid flows is

\[ 0 = -\frac{\partial P}{\partial x} + \frac{1}{\nu} \frac{\partial^2 v}{\partial z^2}, \quad (26) \]

where \( \nu \) and \( P \) are the fluid viscosity and pressure. If the pressure gradient occurs only at one edge of channel with its length is namely \( L_x \), one can solve the equation using boundary condition \( v(z = -L/2) = v(z = L/2) = 0 \). Then fluid velocity in the parallel plate is given by,

\[ v(z) = \frac{1}{2\nu} \frac{\Delta P}{L_x} \left[ z^2 - \frac{L^2}{4} \right]. \quad (27) \]

Note that the velocity distribution is parabolic in \( z \) variable and called a Poiseuille flow.

The EOM for the DNA dynamics is then given by,

\[ \frac{\partial^2 \Phi}{\partial t^2} - \frac{\partial^2 \Phi}{\partial x^2} - U^2(z)\Phi + \lambda\Phi^3 = 0, \quad (28) \]
where $U^2(z) = m^2_\Phi + 2g^2v^2(z)$. By solving the boundary value problem of fluid velocity, the solution is given by Eqs. (14) and (16) for $\lambda > 0$ and $\lambda < 0$ respectively.

4. Summary

A new model for DNA dynamics immersed in fluid system has been introduced. The model is constructed within the gauge field theory framework to describe the interactions between DNA matter and surrounding fluid from the first principle. The dynamics is then studied for various types of fluid velocity.

The basic behavior of the bubble dynamics is described by a pulse solitary waves in Eq. (16). The open state dynamics, that is usually described by the soliton solution, in the present model is realized in the case of uniform fluid velocity as depicted in Fig. 2. The open bubble should correspond to the nonlinear excitation, and thus it is induced by the nonlinear dynamics of DNA double helix itself. From the figure, one can conclude that the bubble amplitude is getting greater as the fluid flows at a constant velocity. On the other hand, the dotted line represents the effects of torsional motion on the DNA immersed in the oscillating fluid, i.e. $v = \sin(\omega x)$. However, the oscillation in the bubble dynamics is relatively small.
Fig. 3. The rotational motion of DNA in term of a pulse solitary wave in the Poiseuille flow with a fixed parameter set \((m_\Phi, v, C, \lambda) = (1, 5, 0.5, 0.2)\) since by assumption the perturbation term (fluid velocity) is kept small.

Another effects due to stratified flow in the bubble dynamics is shown in Fig. 3. As mentioned above, according to the experiments the average extension of DNA under shear flow was found to increase gradually with increasing velocity gradient, reaching a plateau below half-full extension. The hydrodynamics friction is more important factor to aligned of the DNA molecule in a direction parallel to the flow. The present result is given in Fig. 3 which shows that the fluid flow increases the soliton amplitude with the same profile, that is it reaches the peak at the center and almost unaffected near the plateau.

Further, the effects of external forces like electromagnetic force might be interesting to be investigated. This might be important as one considers the nanofluidic system. This will be worked out and discussed in the next-coming works.

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References

1. L. V. Yakushevich, *Nonlinear physics of DNA 2nd edn* (Wiley and Sons, 2002).
2. L. V. Yakushevich, A. V. Savin and L. I. Mawvich, *Phys. Rev. E* **66**, p. 016614 (2002).
3. D. Voet, J. G. Voet and C. W. Pratt, *Fundamental of Biochemistry* (John Wiley and Son, 2008).
4. S. Zdrakovici, J. A. Tuszynski and M. V. Sataric, *J. Comput. Theor. Nanosci*, **21**, 1 (2005).
5. J. P. Rickgauer and D. E. Smith, *Single-Molecule Studies of DNA* (Kluwer Academic Pub., 2006), ch. Soft Matter: Scattering, Imaging and Manipulation.
6. A. Sulaiman and L. T. Handoko, *J. Comp. Theor. Nanosci.* 8, 124 (2011).
7. A. Sulaiman, A. Fajaruddin, T. P. Djun and L. T. Handoko, *Int. J. Mod. Phys. A*, 24, 3630 (2009).
8. L. H. Ryder, *Quantum Field Theory 2nd Ed.* (Cambridge University Press, 1996).
9. F. Cooper, A. Khare, B. Mihaila and A. Saxena, *Phys. Rev. E* 72, p. 036605 (2005).
10. M. W. Dingemans, *Water Waves Propagation over Uneven Bottom* (World Scientific, 1997).
11. M. Cadoni, R. D. Leo and S. Demelio, *Int. J. Non-linear Mechanics* 43, p. 1094 (2009).
12. J. Viovy, *Rev. Mod. Phys.* 72, 813 (2000).