# Employment of Jacobian elliptic functions for solving problems in nonlinear dynamics of microtubules*

Slobodan Zeković[a], Annamalai Muniyappan[b], Slobodan Zdravković[a)†], and Louis Kavitha[b)c)]

[a)] *Institut za nuklearne nauke Vinča, Laboratorija za atomsku fiziku* 040, *Univerzitet u Beogradu, Poštanski fah* 522, 11001 *Beograd, Serbia*
[b)] *Department of Physics, Periyar University, Salem*-636 011, *Tamilnadu, India*
[c)] *Center for Nanoscience and Nanotechnology, Periyar University, Salem*-636 011, *Tamilnadu, India*

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We show how Jacobian elliptic functions (JEFs) can be used to solve ordinary differential equations (ODEs) describing the nonlinear dynamics of microtubules (MTs). We demonstrate that only one of the JEFs can be used while the remaining two do not represent the solutions of the crucial differential equation. We show that a kink-type soliton moves along MTs. Besides this solution, we also discuss a few more solutions that may or may not have physical meanings. Finally, we show what kind of ODE can be solved by using JEFs.

**Keywords:** Jacobian elliptic functions, ordinary differential equations, microtubules, kink soliton

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## 1. Introduction

Microtubules (MTs) are important cell proteins. They represent cytoskeletal structures and serve as a "road network" for motor proteins (kinesin and dynein) dragging different molecular cargos. They are hollow tubes with an inner and outer diameter of 17 nm and 25 nm, respectively.[1]

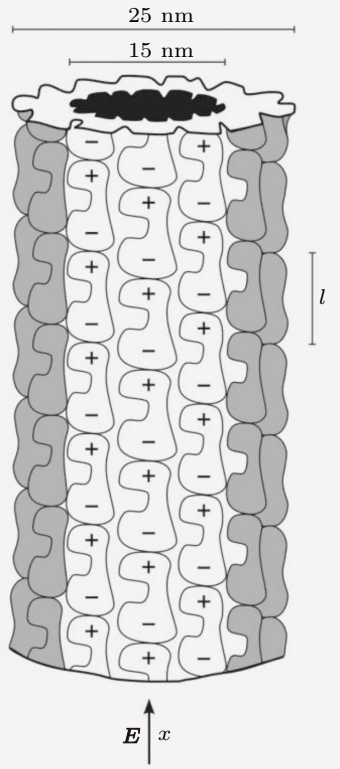



**Fig. 1.** Structure of a microtubule.

Its length may span dimensions from the order of micrometers to the order of millimeters. The cylindrical wall is usually formed by 13 longitudinal structures called protofilaments (PFs), as shown in Fig. 1. They are a series of proteins known as tubulin dimers.[2,3] Each dimer is an electric dipole whose length and longitudinal component of the electric dipole moment are $l = 8$ nm[2–4] and $p = 337$ deb (1 deb $= 3.33564 \times 10^{-30}$ C·m),[5,6] respectively. The constituent parts of the dimers are $\alpha$ and $\beta$ tubulins, corresponding to positively and negatively charged sides, respectively.[2–4]

The rest of this paper is organized as follows. In Section 2, we briefly review one of the models describing MT dynamics. As is well known, for a travelling wave, a partial differential equation (PDE) can be transformed into ODE. This equation, crucial for the model, is solved using JEFs in Section 3. We do believe that this method is the simplest and the most elegant of all. A couple of solutions of the mentioned equation that may or may not have physical meanings are studied in Section 4. In Section 5, we show what kind of ODE can be solved using JEFs. Finally, concluding remarks are presented in Section 6.

## 2. *Z*-model of MTs

In the model, per dimer is assumed to have only one degree of freedom, that is, $z_n$, a longitudinal displacement of a dimer at a position $n$ in a direction of PF, which is the direction of $x$ axes. Hence, we refer to the model as a $z$-model.[7] In what follows, we very briefly describe the model. Of crucial importance is the fact that the bonds between dimers within the same

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†Corresponding author. E-mail: szdjidji@vinca.rs

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PF are much stronger than the soft bonds between neighboring PFs.[8,9] This implies that the longitudinal displacements of pertaining dimers in a single PF should cause the longitudinal wave propagating along PF. All this means that we can write the Hamiltonian for one PF only and express it as[7]

$$H=\sum_n\left[\frac{m}{2}\dot{z}_n^2+\frac{k}{2}\left(z_{n+1}-z_n\right)^2+V(z_n)\right], \tag{1}$$

where dot means the first derivative with respect to time, $m$ is the mass of the dimer and $k$ is a harmonic constant describing the nearest-neighbor interaction between the dimers belonging to the same PF. The first two terms on the right-hand side in Eq. (1) are the kinetic energy of the dimer and harmonic energy, respectively. The latter one is an elastic energy, which is a potential energy of the chemical interaction between the neighboring dimers belonging to the same PF. The last term in Eq. (1) is the combined potential

$$V(z_n)=-Cz_n-\frac{1}{2}Az_n^2+\frac{1}{4}Bz_n^4,\quad C=qE, \tag{2}$$

where $E$ is the magnitude of the intrinsic electric field while $q$ is the excess charge within the dipole. It is assumed that $q>0$ and $E>0$. The first term on the right-hand side in Eq. (2) is an energy of the dimer at the site $n$ in the field $E$ and the remaining two represent the well-known double-well potentials with positive parameters $A$ and $B$ that should be determined.[10] The double-well potential is rather common in physics.[11–14] The first attempt to use it in nonlinear dynamics of MTs was done about 20 years ago.[10,15]

From Eqs. (1) and (2), assuming a continuum approximation $z_n(t)\to z(x,t)$, we straightforwardly obtain the following nonlinear PDE of motion:

$$m\frac{\partial^2 z}{\partial t^2}-kl^2\frac{\partial^2 z}{\partial x^2}-qE-Az+Bz^3+\gamma\frac{\partial z}{\partial t}=0, \tag{3}$$

where the last term represents a viscosity force with $\gamma$ being a viscosity coefficient.[7,10] For a travelling wave $z(x,t)=z(\xi)$, PDE (3) transforms into an ordinary differential equation[7,10]

$$\alpha\psi''-\rho\psi'-\psi+\psi^3-\sigma=0, \tag{4}$$

where $\psi'\equiv \mathrm{d}\psi/\mathrm{d}\xi$,

$$\alpha=\frac{m\omega^2-kl^2\kappa^2}{A},\quad \rho=\frac{\gamma\omega}{A},\quad \sigma=\frac{qE}{A\sqrt{A/B}} \tag{5}$$

and

$$z=\sqrt{\frac{A}{B}}\,\psi. \tag{6}$$

The unified variable $\xi$ is

$$\xi=\kappa x-\omega t, \tag{7}$$

where $\kappa$ and $\omega$ are constants.

A standard way of solving Eq. (4) is rather tedious.[10,12] A more elegant and relatively new procedure is the modified extended tanh-function (METHF) method.[16–21] In the next section, we demonstrate the elegance of the method based on JEFs.

## 3. Jacobian elliptic functions

As stated above, the main purpose of this work is to study whether and how JEFs can be used to solve biophysical problems. In particular, we demonstrate the usefulness of these functions in solving Eq. (4).

Properties of JEFs $\mathrm{sn}(\beta\xi)$, $\mathrm{cn}(\beta\xi)$ and $\mathrm{dn}(\beta\xi)$ with the modulus $m$ can be found in many textbooks and papers.[22–26] A basic algebra includes the following formulae:

$$\mathrm{sn}^2(x)+\mathrm{cn}^2(x)=1,\quad \mathrm{dn}^2(x)=1-m^2\mathrm{sn}^2(x), \tag{8}$$

and

$$\left.\begin{aligned}\mathrm{sn}'(x)&=\mathrm{cn}(x)\,\mathrm{dn}(x)\\ \mathrm{cn}'(x)&=-\mathrm{sn}(x)\,\mathrm{dn}(x)\\ \mathrm{dn}'(x)&=-m^2\,\mathrm{sn}(x)\,\mathrm{cn}(x)\end{aligned}\right\}, \tag{9}$$

where prime denotes the first derivative. When $m\to 1$, the JEFs degenerate into hyperbolic functions, that is,

$$\left.\begin{aligned}\mathrm{sn}(x)&\to\tanh(x)\\ \mathrm{cn}(x)&\to\mathrm{sec\,h}(x)\\ \mathrm{dn}(x)&\to\mathrm{sec\,h}(x)\end{aligned}\right\}. \tag{10}$$

Also, for $m\to 0$, these functions degenerate into trigonometric functions, which is, however, not relevant to this paper.

Our ansatz is the following function:

$$\psi=a_0+\sum_{i=1}^{M}\left(a_i\Phi^i+b_i\Phi^{-i}\right), \tag{11}$$

where $\Phi=\Phi(\xi)$ is one of the JEFs. We start with the function

$$\Phi=\mathrm{sn}(\beta\xi), \tag{12}$$

where $\beta$ is a parameter to be determined. The highest orders of the function $\Phi$ in the expressions for $\psi''$ and $\psi^3$ are $\Phi^{M+2}$ and $\Phi^{3M}$ respectively, which brings about $M=1$. Using Eqs. (8) and (9) we can easily show that the second derivative $\psi''$ can be expressed in terms of $\Phi$, while the first one is proportional to $\mathrm{cn}(\beta\xi)\,\mathrm{dn}(\beta\xi)$. This term can be expressed through $\Phi$ only for $m=1$. Hence, for $M=1$ and $m=1$, we come up with

$$\psi=a_0+a_1\Phi+b_1\Phi^{-1}, \tag{13}$$

$$\psi'=\beta\left(a_1-a_1\Phi^2+b_1-b_1\Phi^{-2}\right) \tag{14}$$

and

$$\psi''=2\beta^2\left(a_1\Phi^3-a_1\Phi-b_1\Phi^{-1}+b_1\Phi^{-3}\right), \tag{15}$$

where

$$\Phi=\tanh(\beta\xi), \tag{16}$$

which comes from Eqs. (10) and (12).

If we plug the expressions for $\psi$, $\psi'$, $\psi''$, and $\psi^3$ into Eq. (4), then we obtain the crucial Eq.

$$A_1\Phi + B_1\Phi^{-1} + A_2\Phi^2 + B_2\Phi^{-2} + A_3\Phi^3 + B_3\Phi^{-3} + A_0 = 0, \tag{17}$$

where the following set of abbreviations is used:

$$A_0 = -a_0 + a_0^3 + 6a_0a_1b_1 - \rho\beta a_1 - \rho\beta b_1 - \sigma, \tag{18}$$
$$A_1 = -a_1 + 3a_0^2a_1 + 2\alpha\beta^2a_1 + 3a_1^2b_1, \tag{19}$$
$$B_1 = -b_1 + 3a_0^2b_1 - 2\alpha\beta^2b_1 + 3a_1b_1^2, \tag{20}$$
$$A_2 = 3a_0a_1^2 + \rho\beta a_1, \tag{21}$$
$$B_2 = 3a_0b_1^2 + \rho\beta b_1, \tag{22}$$
$$A_3 = 2\alpha\beta^2a_1 + a_1^3, \tag{23}$$

and

$$B_3 = 2\alpha\beta^2b_1 + b_1^3. \tag{24}$$

Of course, Eq. (17) is satisfied if all these coefficients are simultaneously equal to zero, which yields a system of seven equations. The solutions expressed through hyperbolic cotangent are not biophysically tractable as this function diverges. This means that we are looking for the acceptable solutions for which $a_1 \neq 0$ and $b_1 = 0$. A more general case is studied in Section 4. Hence, we deal with the system of four equations only and its solution, i.e., the values of the parameters $\beta$, $a_0$, $a_1$ and $\alpha$, which are given through

$$8a_0^3 - 2a_0 + \sigma = 0, \tag{25}$$
$$a_1^2 = 1 - 3a_0^2, \tag{26}$$
$$\rho\beta = -3a_0a_1 \tag{27}$$

and

$$2\alpha\beta^2 = -a_1^2. \tag{28}$$

Notice that $\alpha < 0$ and that there should be

$$a_0^2 < \frac{1}{3} \tag{29}$$

for $a_1$ to be real.

The polynomial (25) has three real roots for[27]

$$\sigma < \sigma_0 = \frac{2}{3\sqrt{3}}. \tag{30}$$

These solutions, as shown in Fig. 2, are

$$a_{01} = \frac{1}{2\sqrt{3}}\left(\cos F + \sqrt{3}\sin F\right), \tag{31}$$
$$a_{02} = \frac{1}{2\sqrt{3}}\left(\cos F - \sqrt{3}\sin F\right), \tag{32}$$
$$a_{03} = -\frac{1}{\sqrt{3}}\cos F, \tag{33}$$

where

$$F = \frac{1}{3}\arccos\left(\frac{\sigma}{\sigma_0}\right). \tag{34}$$

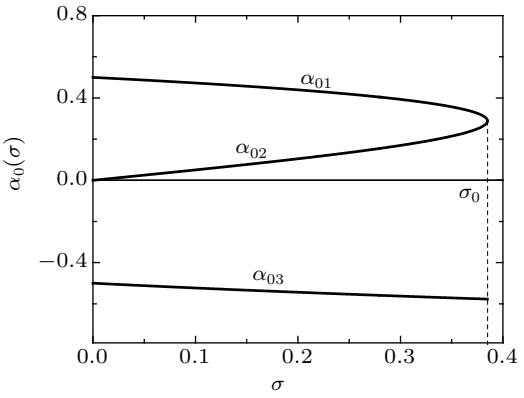



**Fig. 2.** Values of $a_0$, each as a function of parameter $\sigma$.

According to Eqs. (13), (26), and (27), we easily obtain the following solutions of Eq. (4) for $b_1 = 0$

$$\psi_k(\xi) = a_{0k} - \sqrt{1 - 3a_{0k}^2}\tanh\left(\frac{3a_{0k}}{\rho}\sqrt{1 - 3a_{0k}^2}\,\xi\right), \quad k = 1,2,3. \tag{35}$$

These are, obviously, kink-type solitons, as shown in Fig. 3. We can see that the functions $\psi_k(\xi)$ depend on $\rho$ and $\sigma$ as the parameters $a_{0k}$ depend on $\sigma$. The solitonic width, i.e., its slope, depends on both $\rho$ and $\sigma$, while the jumps of the functions $\psi_k(\xi)$ from $-\infty$ to $+\infty$ depend on $\sigma$ only. Obviously, the solitonic width is proportional to viscosity $\rho$.

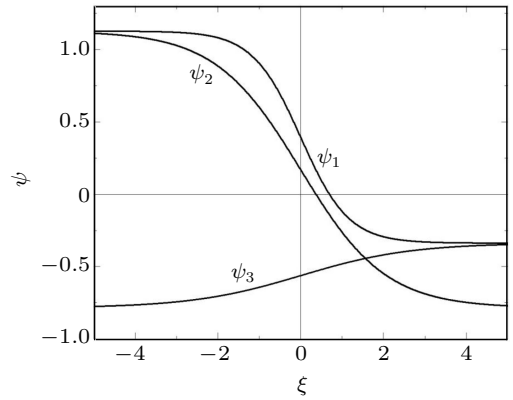



**Fig. 3.** Functions $\psi_k(\xi)$ for $\rho = 1$ and $\sigma = 0.3$.

## 4. Some solutions of Eq. (4) that may not have biophysical meaning

We first investigate the case $\sigma > \sigma_0$. The polynomial given by Eq. (25) has only one real root, which is[28]

$$a_0 = -\frac{1}{\sqrt{3}\sin(2\varphi)}, \quad \tan\varphi = \sqrt[3]{\tan\left[0.5\arcsin\left(\frac{\sigma_0}{\sigma}\right)\right]}, \tag{36}$$

and the solution of Eq. (4) is

$$\psi_t(\xi) = a_0 + \sqrt{3a_0^2 - 1}\,\tan\left(\frac{3a_0}{\rho}\sqrt{3a_0^2-1}\,\xi\right). \quad (37)$$

Of course, the problem with this solution is the fact that the tangent diverges. However, this does not necessarily mean that the solution given by Eq. (37) does not have any physical meaning at all. As is well known, MT is an extremely unstable structure and we speculated recently that the functions including tangent terms might describe its blow up.[27]

Notice that $1-3a_0^2 < 0$ if $\sigma > \sigma_0$. This means that both $a_1$ in Eq. (26) and $\beta$ in Eq. (27) are imaginary and, to derive Eq. (37), a formula $\tanh(\mathrm{i}x) = \mathrm{i}\tan x$ is used.

Our next task is to solve the system of Eqs. (18)–(24) in general, i.e., for $a_1 \neq 0$ and $b_1 \neq 0$. One can easily show that the system reduces into five equations. The solution of this system is given by

$$4a_1^2 = 1 - 3a_0^2, \quad (38)$$

$$a_1 = b_1, \quad (39)$$

and by Eqs. (25), (27), and (28), the final result is

$$\psi_{kn}(\xi) = a_{0k} - \sqrt{1-3a_{0k}^2}\coth\left(\frac{3a_{0k}}{\rho}\sqrt{1-3a_{0k}^2}\,\xi\right), \quad k = 1,2,3. \quad (40)$$

The next step is to study whether the remaining two JEFs can be used for the solution of Eq. (4). We can easily see that all the terms except $\psi'$ are powers of either cn or dn functions. However, the first derivative $\psi'$ cannot be expressed like this for any value of the modulus $m$. This, certainly, means that sn is the only choice for the solution of Eq. (4).

## 5. General case

Equations like Eq. (4) appear rather often. Now we mention just one more example. The model where only longitudinal displacements of dimers are taken into consideration is described in Section 2. If per dimer is assumed to have one radial degree of freedom, we can use the potential energy $-\boldsymbol{p}\cdot\boldsymbol{E} = -pE\cos\varphi$ instead of the one given by Eq. (2), where $\boldsymbol{p}$ and $\boldsymbol{E}$ are a moment of the electric dipole and electric field strength, respectively. Hence, $\sin\varphi$ appears in Eq. (3) and a series expansions brings about terms $\varphi$ and $\varphi^3$. Finally, instead of Eq. (4) we obtain[29]

$$\alpha\psi'' - \rho\psi' + \psi - \psi^3 = 0. \quad (41)$$

It is obvious that Eq. (41) is simpler than Eq. (4) which, of course, can be solved using the same method as above. Therefore, it is extremely important to know what kind of ODE can be solved using JEFs, which is the topic of this section.

Assume that the equation to be solved is

$$\alpha_1\psi^{(n)} + \alpha_2\psi^{(n-1)} + \cdots + \beta_1\psi^N + \beta_2\psi^{N-1} + \cdots + C = 0, \quad (42)$$

representing an extension of Eq. (4), where $\psi^{(n)}$ is the $n$-th derivative with respect to $\xi$ and $\alpha_i$, $\beta_i$ and $C$ are real constants. The highest orders of the function $\Phi$ in the expressions for $\psi^{(n)}$ and $\psi^N$ are $\Phi^{M+n}$ and $\Phi^{NM}$, respectively. If the highest derivative is the second one, like above, we come up with $M+2 = NM$. This means that the methods explained in the previous two sections can be used only for the two cases. These are $N = 3\,(M = 1)$ and $N = 2\,(M = 2)$. If the highest derivative is $n$, we easily obtain

$$M = \frac{n}{N-1}, \quad (43)$$

representing a combination of the integers. For example, if the highest power is 5, then the methods can be used if $n$ is a multiple of $N-1 = 4$. In other words, the values $n = 4, 8, 12, \ldots$ require the series expansions with $M = 1, 2, 3, \ldots$, respectively. Of course, the modulus $m = 1$ is assumed.

## 6. Conclusions

In this paper, we investigated the nonlinear dynamics of the microtubulin system by invoking an analytical method based on one of the JEFs. The method is very simple and powerful but, like other methods, cannot be used to solve any ODE. We explain how we can know whether the method can be used or not.

For the example studied in this paper, the solutions are given by Eqs. (30)–(35) and by Fig. 3. To understand their meanings better, we should keep in mind that the potential given by Eq. (2) is nonsymmetrical, having two minima. The asymptotic values of the functions $\psi_k(\xi)$ are

$$\left.\begin{array}{ll} \psi_1(-\infty) = \psi_{\min 1}, & \psi_1(+\infty) = \psi_{\max} \\ \psi_2(-\infty) = \psi_{\min 1}, & \psi_2(+\infty) = \psi_{\min 2} \\ \psi_3(-\infty) = \psi_{\min 2}, & \psi_3(+\infty) = \psi_{\max} \end{array}\right\}. \quad (44)$$

Hence, these functions represent transitions from the minimum to the maximum and from a minimum to other minimum. From the physical point of view, we believe that the best solution is $\psi_1(\xi)$. Namely, we expect the system to be in a deeper minimum, denoted as min1, which is a ground state. When a dimer obtains a portion of energy, it may move to the second minimum or to the maximum. In the first case, one more part of the energy would be required for the system to return to the initial ground state. On the other hand, if the system is around its maximum, it can spontaneously return to the deeper minimum.

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