

## Microtubules: Montroll's kink and Morse vibrations

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Using a version of Witten's supersymmetric quantum mechanics proposed by Caticha [Phys. Rev. A **51**, 4264 (1995)], we relate Montroll's kink to a traveling, asymmetric Morse double-well potential, suggesting in this way a connection between kink modes and vibrational degrees of freedom along microtubules. [S1063-651X(97)05901-1]

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Two decades ago, Collins, Blumen, Currie, and Ross [1] studied the dynamics of domain walls in ferrodistorptive materials. They started with a Ginzburg-Landau Hamiltonian (free energy) with driven field and dissipation included leading to the Euler-Lagrange dimensionless equation of motion

$$\psi'' + \rho \psi' - \psi^3 + \psi + \sigma = 0, \quad (1)$$

where the primes are derivatives with respect to a traveling coordinate  $\xi = x - v_K t$ ,  $\rho$  is a friction coefficient, and  $\sigma$  is related to the driven field [1]. This equation is a traveling coordinate transform of a nonlinear reaction-diffusion equation widely studied in the contexts of population genetics and nonequilibrium chemical systems. It has also drawn the attention of pure mathematicians who proved many general results.

Montroll [2] showed that Eq. (1) has a unique bounded (kinklike) solution as follows:

$$\psi(\xi) = a + \frac{b-a}{1 + \exp(\beta\xi)}, \quad (2)$$

where  $\beta = (b-a)/\sqrt{2}$  and the parameters  $a$  and  $b$  are two of the solutions of the cubic equation

$$(\psi - a)(\psi - b)(\psi - d) = \psi^3 - \psi - \sigma. \quad (3)$$

Recently, Montroll's kink has been used as an energy-transfer mechanism in microtubules [3,4] and it is to this particularly interesting biological context that we would like to apply our remarks in the following. But first, it is essential to notice that Montroll's kink can be written as follows:

$$\psi(\xi) = \frac{\beta}{\sqrt{2}} \left[ \left( 1 + \frac{a\sqrt{2}}{\beta} \right) - \tanh\left(\frac{\beta\xi}{2}\right) \right] \quad (4)$$

and an obvious rescaling leads to the useful form

$$K(\xi) = \gamma - \tanh\left(\frac{\beta\xi}{2}\right), \quad (5)$$

where  $\gamma = 1 + a\sqrt{2}/\beta$ . Equation (5) is a requisite in order to enter a construction method of exactly soluble double-well

potentials in the Schrödinger equation proposed by Caticha [5]. The scheme is a nonstandard application of Witten's supersymmetric quantum mechanics [6] having as the essential assumption the idea of considering the kink as the switching function between the two lowest eigenstates of the Schrödinger equation with a double-well potential. Thus

$$\phi_1 = K \phi_0, \quad (6)$$

where  $\phi_{0,1}$  are solutions of  $\phi''_{0,1} + [\epsilon_{0,1} - u(\xi)]\phi_{0,1} = 0$ , and  $u(\xi)$  is the double-well potential to be found. Substituting the assumption Eq. (6) into the Schrödinger equation for the subscript 1 and subtracting the same equation multiplied by the switching function for the subscript 0, one obtains

$$\phi'_0 + W \phi_0 = 0, \quad (7)$$

which is the basic equation introducing the superpotential  $W$  in Witten's supersymmetric quantum mechanics. In the present approach  $W$  is given by

$$W = \frac{K'' + \epsilon K}{2K'}, \quad (8)$$

where  $\epsilon = \epsilon_1 - \epsilon_0$  is the lowest energy splitting in the double-well Schrödinger equation. The ground-state wave function is of the supersymmetric type

$$\phi_0(\xi) = \phi_0(0) \exp\left[-\int_0^\xi W(y) dy\right], \quad (9)$$

where  $\phi_0(0)$  is a normalization constant. The double-well potential is determined up to an additive constant by the "bosonic" Riccati equation

$$u(\xi) = W^2 - W' + \epsilon_0, \quad (10)$$

which is another basic supersymmetric formula. For Montroll's kink the superpotential will be

$$W(\xi) = -\beta \tanh(\beta\xi) + \frac{\epsilon}{4\beta} [\sinh(2\beta\xi) + 2\gamma \cosh^2(\beta\xi)] \quad (11)$$

and the ground-state Schrödinger function reads

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$$\phi_0(\xi) = \phi_0(0) \cosh(\beta\xi) \exp \left[ -\frac{\epsilon}{4\beta^2} \sinh^2(\beta\xi) + \gamma\beta\xi + \frac{\gamma}{2} \sinh(2\beta\xi) \right], \quad (12)$$

while  $\phi_1$  is obtained by switching the ground-state wave function with the kink. If, as suggested by Caticha, one chooses the ground-state energy to be

$$\epsilon_0 = -\beta^2 - \frac{\epsilon}{2} + \frac{\epsilon^2}{32\beta^2} (\gamma^2 - 1), \quad (13)$$

then  $u(\xi)$  is a traveling, asymmetric Morse double-well potential of depths

$$U_0^{L,R} = 4\beta^2 \left[ 1 \pm \frac{2\epsilon\gamma}{(4\beta)^2} \right], \quad (14)$$

where the superscripts stand for left and right well. The difference in depth, the bias, is  $\Delta \equiv U_0^L - U_0^R = 2\epsilon\gamma$ , while the location of the potential minima on the traveling axis is at

$$\xi_{L,R} = \mp \frac{1}{2\beta} \ln \left[ \frac{(4\beta)^2 \pm 2\epsilon\gamma}{\epsilon(\gamma \mp 1)} \right]. \quad (15)$$

Thus, there are two interpretations of the kink in Eq. (5), either as a propagating domain wall through a sequence of on-site quartic double-well potentials, or as a kink connected to a propagating vibrational Morse double well. The latter picture is closer to the spirit of bioenergetics if one remembers the Davydov model where both the vibrational soliton and the phonon kink are of course propagating objects. The Morse double-well picture, though quite appealing, occurs only when the set of relationships Eqs. (13)–(15) is fulfilled by the parameters of the kink and the Morse parameters and therefore some experimental evidence is required. As discussed in [3], in the static on-site picture, the mobile electron on each dimer unit may be localized either more toward the

$\alpha$  monomer or more toward the  $\beta$  one, and in fact the kink is just contributing to the electron tunneling between the two states of the double-well on-site potential. Thus, in the case of the Morse picture, one may think of molecular photoelectron spectroscopy of tubulin dimers performed with a simple retarding-field photoelectron spectrometer, similar, for example, to that of Price and Ibrahim [7]. Moreover, a Morse double-well parametrization of the potential curves corresponding to the differential photoelectron spectrum should be performed. As far as I know, there are no such experimental data at the present time. I recall that in elaborating a Fröhlich-like (coherent) model of microtubules, Samsonovich, Scott, and Hameroff [8] quoted only two *indirect* experimental evidence for the existence of coherent excitations along microtubules, namely, the 2.45 GHz irradiation experiment of Neubauer *et al.* [9] and the microtubule associated protein attachment site superlattices on microtubules [10].

In conclusion, according to Caticha's scheme, experimental evidence of Morse-type vibrations would support both a *traveling* Morse double-well potential and the existence of a (traveling) kink in microtubules with the parameters of the kink depending on the Morse parameters. On the other hand, the same kink parameters may be interpreted in terms of the parameters of a quartic double-well on-site potential (the original Montroll's kink). In other words, if one of the interpretations fails, the kink is still there, while if both are correct further insights into their connection must be provided.

The supersymmetric method is quite general and can be applied to other kinks as well, and as a matter of fact, to any model where a traveling potential is preferred. The weak point is that the ground-state energy should be fixed rather arbitrarily for each case in terms of the kink parameters  $\beta$  and  $\gamma$  and the tunneling splitting  $\epsilon$ .

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