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Physics Letters A 335 (2005) 408–416
PHYSICS LETTERS A
www.elsevier.com/locate/pla

States and properties of the soliton transported bio-energy in nonuniform protein molecules at physiological temperature

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Received 20 July 2004; received in revised form 23 December 2004; accepted 29 December 2004

Available online 7 January 2005

Communicated by R. Wu

Abstract

We have numerically studied states and properties of the soliton transported bio-energy at physiological temperature 300 K by the Runge–Kutta way and dynamic equations in the improved Davydov theory. We proved that the new solitons can move without dispersion retaining its shape and energy in both uniform and nonuniform protein molecules. If considering further effect of thermal perturbation of heat bath on the soliton in the nonuniform proteins, it is still thermally stable at the biological temperature 300 K and in the longer times of 300 ps and larger spacings of 400 amino acids, which is consistent with the analytic result obtained by a quantum perturbed theory. These results exhibit that the new soliton is a possible carrier of the bio-energy transport and the improved model is possibly a candidate for the mechanism of this transport.

PACS: 87.15.He; 36.20.-r

Keywords: Bio-energy transport; Soliton; Protein; Numerical simulation

As known, the bio-energy transport in protein molecules is a very important problem in biology, many biological processes and phenomena need be provided with the energy, for example, the muscle contraction, DNA reduplication and neuroelectric pulse transfer on the neurolemma and work of calcium pump and sodium pump, and so on. The biological energy comes mainly from the hydrolysis reaction of adenosine triphosphate (ATP). How does the bio-energy transport in the living systems? A lot of studies show that the transport in the protein molecules could be carried out by a soliton mechanism [1–15]. The the-

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0375-9601/$ – see front matter
doi:10.1016/j.physleta.2004.12.079

ory of this transport was firstly proposed by Davydov [1]. Following Davydov's idea [1], the soliton is formed through self-trapping of the exciton, a vibrational quantum of amide-I ($C=0$ stretching vibration) arising from the energy released in the ATP hydrolysis, interacting with vibration of amino acid molecules in the α-helix protein. The soliton model of the bioenergy transport is surely a competing picture for the mechanism and consequently has been a subject of a large body of work [2–15]. A lot of problems related to the Davydov model have been extensively studied [2–15]. However, there continues to be considerable controversy concerning the Davydov soliton mechanism in the α-helix protein up to now [7–15]. An elementary question of the controversy is whether the Davydov soliton has a lifetime at the biological temperature 300 K that is sufficiently long for it to play an important part in the living processes. It is out of question that the thermal perturbation and structure disorder are expected to cause the Davydov soliton with one-quantum state to decay into delocalized states. Therefore some have doubted its thermal stability at 300 K [11–15]. The result obtained by quantum Monte Carlo simulation [12] show that the correlations characteristic of the Davydov soliton like quasi-particles only occurred at low temperature about $T<10$ K for widely accepted parameter values. Cottingham et al. [13] obtained also that the lifetime of the Davydov soliton at 300 K is too small (about 10^{-12}–10^{-13} s) to be useful in biological processes by using straightforwardly quantum-mechanical perturbation calculation. This shows that the Davydov solution is not a true wave function of the systems. Thus, a lot of corrections to this model were proposed [5,9–11], but are not successful. Pouthier et al. [17] worked in a modified Davydov model in which the influence of the intramolecular anharmonicity and the strong vibron–phonon coupling on the two-vibron dynamics in the proteins was studied, the vibron dynamics is described according to the small polaron approach. Studies for the relaxation channels of two-vibron bound states shows that the relaxation rate does not significantly depend on the nature of the two-vibron states involved in the process at biological temperature, the lifetime for both bound and free states is of same order of magnitude and ranges between 0.1 and 1.0 ps for realistic parameter values. This is interesting result.

We recently improved [18] the Davydov model. A new interaction between the acoustic vibration of the amino acid and amide-I was added in the Davydov's Hamiltonian, the exciton state with one-quantum in the Davydov's wave function was replaced by the quasi-coherent two-quantum state. They are, respectively,

$$\begin{aligned} H &= H_{\mathrm{ex}} + H_{\mathrm{ph}} + H_{\mathrm{int}} \\ &= \sum_n \left[\varepsilon_0 B_n^+ B_n - J\left(B_n^+ B_{n+1} + B_n B_{n+1}^+\right)\right] \\ &\quad + \sum_n \left[\frac{P_n^2}{2M} + \frac{1}{2}W(u_n - u_{n-1})^2\right] \\ &\quad + \sum_n \left[\chi_1(u_{n+1} - u_{n-1}) B_n^+ B_n \right. \\ &\quad \left. + \chi_2(u_{n+1} - u_n)\left(B_{n+1}^+ B_n + B_n^+ B_{n+1}\right)\right], \end{aligned} \tag{1}$$

$$\begin{aligned} \left|\Phi(t)\right\rangle &= \frac{1}{\lambda}\left[1 + \sum_n a_n(t) B_n^+ \right. \\ &\quad \left. + \frac{1}{2!}\left(\sum_n a_n(t) B_n^+\right)^2\right]|0\rangle_{\mathrm{ex}} \\ &\quad \times \exp\left\{-\frac{\mathrm{i}}{\hbar}\sum_n \left[q_n(t) P_n - \pi_n(t) u_n\right]\right\}|0\rangle_{\mathrm{ph}}, \end{aligned} \tag{2}$$

where B_n and B_n^+ are annihilation and creation operators of the exciton at the nth site associated with the amide-I oscillator having energy $\varepsilon_0 = 0.205$ eV, J describes the nearest neighboring dipole–dipole interaction of the amide-I vibrational quanta, u_n and P_n are the coordinate and momentum operators of the amino acids in the harmonic lattice, respectively, M is the mass of the amino acid molecule, W is the force constant of the protein molecular chains, χ_1 and χ_2 are two coupled constants related to the interactions between the intramolecular excitations and displacements of neighboring amino acids, they represent modulations of the one-site energy and resonant (or dipole–dipole) interaction energy for the excitons caused by the molecular displacements, respectively. $|0\rangle_{\mathrm{ph}}$ and $|0\rangle_{\mathrm{ex}}$ are the vacuum states of the phonon and exciton, respectively, λ is a normalization constant, we here choose it to be 1. Very obviously, the exciton wave function in Eq. (2) is not an excitation state of single particle, but the quasi-coherent state containing exactly two quanta due to