The quantum lifetime of the Davydov soliton

H. Bolterauer and M. Opper
Institut für Theoretische Physik, Justus-Liebig-Universität Giessen, W-6300 Giessen, Federal Republic of Germany

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Considering an infinite spine in the Alpha-helix, stationary states should be eigenstates of a translational operator. These states should be nonlocalized in contradiction to a localized soliton. The difference in energy between localized and nonlocalized (Bloch) states is due to zero point motion and gives information about the quantum stability of the Davydov soliton. We develop a theory of stationary states and show that only for the limiting case of a classical lattice the product ansatz by Davydov is exact. Finally, we calculate the width of the soliton band to get information on the lifetime of the localized soliton.

1. Introduction

In a series of previous papers we dealt with the biological relevance of the Davydov soliton in the Alpha-helix. We calculated solitons which appear when the excitation mechanism is purely classical and therefore the number of excited amide I quanta is not sharp [1]. Also we developed a theory for a two or more quanta soliton [2] and compared it with the usual one quantum soliton used by all other authors [3-9]. Finally, we discussed the problem of thermal fluctuations [10] and the difficulties which appear by using a classical thermalization scheme [11, 12].

This paper deals with another problem: The quantum stability of the Davydov soliton. The soliton, which was introduced by Davydov to explain the energy transport in the Alpha-helix, seems to be a very classical object. It is a localized state with a creation energy and needs kinetic energy to get it moving. Crucial for the soliton solution is the following product ansatz originally given by Davydov [3]

\[ |\Psi\rangle = |\text{lattice}\rangle |\text{oscillators}\rangle \]

\[ |\text{lattice}\rangle = \exp \left[ \frac{1}{i\hbar} \sum_n (X_n P_n - P_n X_n) \right] |0\rangle \]

\[ |\text{oscillators}\rangle = \sum_m f_m b_m^+ |0\rangle. \]

This ansatz neglects correlations between the two subsystems. To optimize this form in a systematic way we used in [1] the time dependent variational principle, which is just the generalization of the ordinary variation principle of quantum mechanics. This approximation scheme yields equations of motion, which are almost identical with Davydov's equations and have solitons as solutions.

The next question is: Is a product ansatz for this system good enough [13, 14]? We will show in this paper, that only in the limit of a purely classical lattice the ansatz (1.1) is exactly valid. Therefore, we then have to ask how stable the Davydov soliton is against quantum fluctuations and whether the lifetime of the soliton is long enough for biological relevance.

In this paper we assume that the Alpha-helix is long enough so that we can neglect effects coming from the ends of the chain. Therefore we use periodic boundary conditions well known from solid state physics.

The plan of this paper is as follows:

In Chap. 2 we develop a theory of stationary using the symmetry of the Hamiltonian (no lattice site is preferred). It follows that stationary states must have a Bloch form.

In the first part of chapter three, we discuss various limiting cases of the Hamiltonian. Using perturbation theory we calculate the energy band for a small coupling of the two subsystems.

In the second part of Chap. 3 we try to use the well known polaron ansatz of Lee Low and Pines. We show that this ansatz gives poor results, if the lattice, as one of the subsystems, can be considered as classical.

In Chap. 4 we again concentrate our discussion on the case of a classical lattice. We show that this assumption makes the Davydov ansatz exact. The oscillators remain quantized since we are interested in one quantum states.

In the rest of this paper we discuss the important question if the soliton can remain localized even if the lattice is not classical. For simplicity we deal with a non moving Davydov soliton which we can compare with stationary states.
In Chap. 5 we again use methods from solid state physics showing that a delocalization of the soliton wave function will always lower the energy. The so calculated "soliton band" should be seen merely as a tool to calculate the lifetime of the Davydov soliton (1.1). It is not a good approximation for the states if the bandwidth is not small. Better calculations for the band of the Davydov Hamiltonian for this case can be found in [15–18].

In Chap. 6 we calculate the uncertainty in energy and the lifetime of the Davydov soliton. We finish with a discussion of the results in Chap. 7.

2. The equation for stationary states

We start from the Hamiltonian [2, 3]

\[ H = H_L + H_O + H_I \]

\[ H_L = \sum_n \left( \frac{p_n^2}{2M} + \frac{1}{2} K(q_n - q_{n-1})^2 \right) \]

\[ H_O = \sum_n \left[ \varepsilon b_n^+ b_n - J b_n^+ (b_{n+1} + b_{n-1}) \right] \]

\[ H_I = \chi \sum_n b_n^+ b_n (q_n - q_{n-1}) \quad (2.1) \]

\( H_L \) denotes the lattice part and \( H_O \) the amide I oscillators. We immediately see that \( N \), the number of oscillator quanta

\[ N = \sum_n b_n^+ b_n \quad (2.2) \]

is a constant of motion. So, for the eigenstates of \( H \) we can distinguish between zero, one, two and more quantum states. In a mixed representation, where we use a wavefunction for the lattice and a state vector for the oscillators, we can write this in the following form

\[ |\Psi^0\rangle = \varphi(q) |0\rangle \]

\[ |\Psi^1\rangle = \sum_m \varphi(m, q) b_m^+ |0\rangle \]

\[ |\Psi^2\rangle = \sum_{m, m'} \varphi(m, m', q) b_m^+ b_{m'}^+ |0\rangle. \quad (2.3) \]

The zero quantum state \(|\Psi^0\rangle\) is easily calculated since there is no interaction between the two subsystems and

\[ \varphi(q) = \varphi(q_1, q_2, \ldots, q_L) \quad (2.4) \]

represents the well known eigenfunctions of the harmonic lattice.

In the following we want to concentrate on the one quantum state \(|\Psi^1\rangle\). The eigenvalue equation

\[ H |\Psi^1\rangle = E |\Psi^1\rangle \quad (2.5) \]

yields a Schrödinger equation for the wavefunction \( \varphi(m, q) \)

\[ \left[ \sum_n \left( \frac{p_n^2}{2M} + \frac{1}{2} K(q_n - q_{n-1})^2 \right) + \varepsilon + \chi(q_m - q_{m-1}) \right] \varphi(m, q) - J \left[ \varphi(m+1, q) + \varphi(m-1, q) \right] = E \varphi(m, q) \quad (2.6) \]

or

\[ h \varphi(m, q) = E \varphi(m, q) \quad (2.7) \]

with

\[ h = \sum_n \left( \frac{p_n^2}{2M} + \frac{1}{2} K(q_n - q_{n-1})^2 \right) + \varepsilon + \chi(q_m - q_{m-1}) - J (A^+ + A^-). \quad (2.8) \]

Here, the operators \( A^+ \) and \( A^- \) make a shift in \( m \), that is a shift in the oscillator labels.

\[ A^+ \varphi(m, q) = \varphi(m + 1, q), \]

\[ A^- \varphi(m, q) = \varphi(m - 1, q). \]

The interaction term can also be written in the following form

\[ \chi(q_m - q_{m-1}) \varphi(m, q) = \sum_{m'} \chi(q_{m'} - q_{m'-1}) \delta_{m', m} \varphi(m, q) \quad (2.9) \]

where the operator \( \mathcal{M} \) is defined by

\[ \mathcal{M} \varphi(m, q) = m \varphi(m, q). \quad (2.10) \]

The Hamiltonian \( h \) in the Schrödinger equation for \( \varphi(m, q) \) is invariant against a translation of the whole system. To formulate this, we introduce further Operators \( Q^+, Q^- \) which are shifting operators for the lattice labels.

\[ Q^+ \varphi(m, q_1, q_2, q_3 \ldots q_L) = \varphi(m, q_2, q_3 \ldots q_L, q_1) \]

\[ Q^- \varphi(m, q_1, q_2, q_3 \ldots q_L) = \varphi(m, q_L, q_1, q_2 \ldots q_{L-1}). \quad (2.11) \]

Here, and for the following, we assume periodic boundary conditions. We will show now that the total translational operator \( T = A^+ Q^+ \) commutes with \( h \)

\[ [h, T] = 0. \quad (2.12) \]

The only tricky term is the interaction part (2.9). Since for any function \( f(x) \)

\[ A^+ f(\mathcal{M}) = f(\mathcal{M} - 1) A^+ \]

holds, we get

\[ A^+ Q^+ \sum_{m'} (q_{m'} - q_{m'-1}) \delta_{m', m} \varphi(m, q) = Q^+ \sum_{m'} (q_{m'} - q_{m'-1}) \delta_{m', m} A^+ \varphi(m, q) = \sum_{m'} (q_{m'} - q_{m'-1}) \delta_{m', m} A^+ Q^+ \varphi(m, q) \quad (2.13) \]

where

\[ A^+ Q^+ \sum_{m'} (q_{m'} - q_{m'-1}) \delta_{m', m} \varphi(m, q) = \sum_{m'} (q_{m'} - q_{m'-1}) A^+ Q^+ \varphi(m, q) \]