Quantum and temperature effects on Davydov soliton dynamics: averaged Hamiltonian method

1992 J. Phys.: Condens. Matter 4 1915

(http://iopscience.iop.org/0953-8984/4/8/007)

J. Phys.: Condens. Matter 4 (1992) 1915–1923. Printed in the UK

Quantum and temperature effects on Davydov soliton dynamics: averaged Hamiltonian method

Wolfgang Förner
Laboratory of the National Foundation for Cancer Research,
Friedrich-Alexander-University Erlangen-Nürnberg, Egerlandstrasse 3,
D-8520 Erlangen, Federal Republic of Germany

Received 13 September 1991

Abstract. The dynamics of Davydov solitons within the so-called $|D_1\rangle$ state which allows quantum effects in the lattice are studied at physiological temperatues using Davydov's averaged Hamiltonian method. For this purpose the Euler–Lagrange method is used to obtain approximate equations of motion from a thermally averaged Hamiltonian. Within $|D_1\rangle$ dynamics at $T = 0$ K and for parameter values appropriate for proteins, no solitons are found. It is demonstrated that temperature effects at 300 K shift the stability window for travelling solitons into regions of the parameter space which might be realistic for proteins.

1. Introduction

For the mechanism of energy transport through proteins, Davydov [1, 2] suggested that the energy of about 0.4 eV released by the hydrolysis of adenosine-triphosphate (ATP) could be transported in quanta of the amide-I (mainly C=O stretch) vibration (about 0.2 eV). The CO groups participate in hydrogen bonds which form chains parallel to the axis of α-helical proteins. Thus the amide-I vibration interacts with the acoustic phonons in these chains. The excitation of an amide-I oscillator [1, 2] causes a distortion in the lattice which in turn stabilizes the amide-I excitation. It was found that for certain regions of the parameter space of the model this effect can prevent the excitation from dispersion via the dipole–dipole coupling between neighbouring CO groups in the lattice. The region in which the vibrational energy is localized can travel as a soliton along the chain.

In his original theory, Davydov and co-workers [1] used an *ansatz* for the wavefunction ($|D_2\rangle$) which treats the lattice classically. At zero temperature it has been confirmed that Davydov solitons exist for parameter values appropriate for proteins [3]. Also their stability against disorder along the chain was studied [4]. The investigation of temperature led to controversial results. Halding and Lomdahl [5] found stable pulses at $T = 310$ K using classical molecular dynamics for peptide units moving in a Lennard-Jones potential. Lomdahl and Kerr [6] and others [7] used the $|D_2\rangle$ *ansatz* together with a damping and a noise term to introduce temperature and found no stable solitons at 310 K at a specific set of parameters. Bolterauer [8] argued that their classical thermalization scheme might lead to a too large transfer of energy into the quantum system (oscillators). Cottingham and Schweitzer [9] applied perturbation theory to the Hamiltonian after partial diagonalization and could show (again for one set of parameters)

0953-8984/92/081915 + 09 $04.50

that the soliton lifetime at 300 K is too short for biological processes. In our previous work [4, 10, 11] we prepared the lattice in a thermally excited state prior to the soliton start. We compared our results with those of [6] and found agreement between the models if in the Langevin model [6] the lattice is thermally equilibrated before the soliton starts. We could show that, in a window in the parameter space which might well be realistic for proteins, travelling solitons exist at 300 K.

Recently Brown *et al* [12] have shown that the $|D_2\rangle$ state *ansatz* does not reproduce the dynamics of the exactly solvable small-polaron limit (dipole–dipole coupling neglected). Davydov [2] introduced a more sophisticated *ansatz* state ($|D_1\rangle$) which allows for quantum effects in the lattice. However, he used the energy expectation value for $|D_1\rangle$ as the classical Hamiltonian function to derive equations of motion [2]. It was shown that with these equations $|D_1\rangle$ does not reproduce the small-polaron limit [12] either. With these equations of motion and a thermally averaged Hamiltonian, Davydov [2] could show within the continuum limit that solitons exist at 300 K. Cruzeiro *et al* [13] reached the same conclusion numerically without making use of Davydov's approximations.

Most recently Mechtly and Shaw [14] and Skrinjar *et al* [15] could derive new equations of motions for $|D_1\rangle$ with the help of quantum mechanical methods. These equations of motion reproduce the small-polaron limit. However, in the general case also this *ansatz* state is still approximate. In [14] as well as in our work [16] it is shown that at $T = 0$ K the window for travelling solitons in the $|D_1\rangle$ state occurs in regions of the parameter space which cannot be applied to proteins (soliton formation threshold $X > 150$ pN).

2. Method

In this paper we wish to report the results at $T = 300$ K using the $|D_1\rangle$ state *ansatz*. The Hamiltonian [1, 2] including disorder is given by

$$\hat{H} = \sum_n [(E_0 + E_n)\hat{a}_n^+ \hat{a}_n - J_n(\hat{a}_{n+1}^+ \hat{a}_n + \hat{a}_n^+ \hat{a}_{n+1})] + \sum_k \hbar\omega_k \left(\hat{b}_k^+ \hat{b}_k + \tfrac{1}{2} + \sum_n B_{nk}(\hat{b}_k + \hat{b}_k^+)\hat{a}_n^+ \hat{a}_n \right) \tag{1}$$

$$B_{nk} = (X_n/\omega_k)(1/\sqrt{2\hbar\omega_k})(U_{n+1,k}/\sqrt{M_{n+1}} - U_{nk}/\sqrt{M_n}).$$

$\hat{a}_n^+$ and $\hat{a}_n$ are creation and annihilation operators, respectively, for quanta of amide-I oscillators at site n, and $\hat{b}_k^+$ and $\hat{b}_k$ the creation and annihilation operators, respectively, for acoustic phonons of wavenumber k. The translational mode has to be excluded from the summation. E_0 is the excitation energy of a free oscillator (0.205 eV), and E_n a site-dependent deviation from E_0 due to disorder. J_n is the dipole–dipole coupling constant between neighbouring amide-I oscillators (n and $n + 1$). For J, usually 0.967 meV is used. X_n is the coupling constant between the oscillators and the lattice. Note that we use the asymmetric interaction model where only the coupling of the oscillator n to the hydrogen bond between n and $n + 1$ in which the oscillator takes part is considered. For X usually a value of 62 pN is used. M_n are the masses of the amino acids. Here we have applied the average value of $114m_p$ for all sites (m_p is the proton mass), ω_k denotes the

eigenfrequency of the normal mode k and **U** contains the normal mode coefficients. ω and **U** are obtained by numerical diagonilization of the matrix **V** with elements

$$V_{nm} = \{[W_n(1 - \delta_{nN}) + W_{n-1}(1 - \delta_{n1})]\delta_{nm} - W_n(1 - \delta_{nN})\delta_{m,n+1} - W_{n-1}(1 - \delta_{n1})\delta_{m,n-1}\}(M_n M_m)^{-1/2}. \quad (2)$$

The form of **V** implies that we use free chain ends and N units. Other boundary conditions such as cyclic [13] or fixed chain ends [14] would require another form of **V**. W_n is the force constant of the hydrogen bond between sites n and $n + 1$. For W, usually 13 N m^{-1} [17] is applied.

The $|D_1\rangle$ *ansatz* for inclusion of temperature in Davydov's approximation for solution of the time-dependent Schrödinger equation is

$$|D_1, \nu\rangle = \sum_n a'_n(t)\hat{a}_n^+ |0\rangle_e |\beta_n, \nu\rangle. \quad (3)$$

Here $|0\rangle_e$ is the exciton vacuum, and $|\beta_n\rangle$ a coherent phonon state. For the one-quantum oscillator states used here $\Sigma|a_n|^2 = 1$ holds. To include temperature approximately we assume, as in [13], that a phonon distribution

$$|\nu\rangle = \prod_k \frac{1}{\sqrt{\nu_k!}} (\hat{b}_k^+)^{\nu_k} |0\rangle_p \quad (4)$$

is present in the lattice where each normal mode is occupied by ν_k quanta. Here $|0\rangle_p$ is the phonon vacuum. We do not consider a thermal distribution of amide-I quanta since at 300 K the Boltzmann factor implies that only 3 of 10 000 amide-I oscillators would be thermally excited. Thus one can neglect a possible thermalized soliton distribution in the system too, since the presence of solitons requires first of all amide-I excitation. Then

$$|\beta_n, \nu\rangle = \exp\left(\sum_k (b_{nk}(t)\hat{b}_k^+ - b_{nk}^*(t)\hat{b}_k)\right)|\nu\rangle \quad (5)$$

where the $b_{nk}(t)$ are the coherent state amplitudes. Following the derivation of Cruzeiro *et al* [13] (done for cyclic ordered chains) we obtain the thermally averaged Hamiltonian

$$H_T = \sum_n \left((E_0 + E_n)|a'_n|^2 - J_n a'^*_n a'_{n+1} D_{n,n+1} - J_{n-1} a'^*_n a_{n-1} D_{n,n-1} + |a'_n|^2 \sum_k \hbar\omega_k [B_{nk}(b_{nk} + b_{nk}^*) + v_k + |b_{nk}|^2] \right) \quad (6)$$

with (k_B is Boltzmann's constant)

$$v_k = 1/[\exp(\hbar\omega_k/k_B T) - 1] \quad (7)$$

(Bose–Einstein statistics) and

$$D_{nm} = \exp\left(\sum_k [(v_k + 1)b_{nk}^* b_{mk} + v_k b_{nk} b_{mk}^* - (v_k + \tfrac{1}{2})(|b_{nk}|^2 + |b_{mk}|^2)]\right). \quad (8)$$

The equations of motion can be obtained with the Euler–Lagrange formalism [15]

and one obtains finally (see [16])

$$\begin{aligned}
i\hbar\dot{a}_n &= -\frac{i\hbar}{2}a_n\sum_k(\dot{b}'_{nk}b^*_{nk} - \dot{b}'^*_{nk}b_{nk}) + E_n a_n - J_n D_{n,n+1}a_{n+1} \\
&\quad - J_{n-1}D_{n,n-1}a_{n-1} + a_n\sum_k \hbar\omega_k[B_{nk}(b_{nk} + b^*_{nk}) + |b_{nk}|^2] \\
a'_n(t) &= a_n(t)\exp\left[-\frac{i}{\hbar}\left(E_0 + \sum_k \hbar\omega_k v_k\right)t\right] \qquad (9)
\end{aligned}$$

$$\begin{aligned}
i\hbar\dot{b}_{nk} &= \hbar\omega_k(B_{nk} + b_{nk}) \\
&\quad -J_n(b_{n+1,k} - b_{nk})[(v_k + 1)D_{n,n+1}a_{n+1}/a_n + v_k D_{n+1,n}a^*_{n+1}/a^*_n] \\
&\quad -J_{n-1}(b_{n-1,k} - b_{nk})[(v_k + 1)D_{n,n-1}a_{n-1}/a_n + v_k D_{n-1,n}a^*_{n-1}/a^*_n].
\end{aligned}$$

To avoid numerical difficulties due to the denominators a_n and a^*_n we used as initial condition ($N = 50$)

$$a_n(0) = A[\delta_{n,n_0} + x_n(1 - \delta_{n,n_0})] \qquad (10)$$

where A is the normalization constant, $x_n = 0.005$ as in [14] and $n_0 = 49$.

This method introduced by Davydov was criticized by several workers as being inconsistent with quantum mechanics. However, we feel that it might still be a reliable approximation to the real dynamics under physiological temperature. To investigate this we also give a comparison with quantum Monte Carlo simulations below. One can view the 'thermally averaged state' used here as a linear combination of all states with a fixed phonon distribution in the lattice, where the weight factors of the individual states follow Bose–Einstein statistics. In the appendix we outline a modified method using an *ansatz* which overcomes the conceptual difficulties mentioned above. Numerical results from this modified method will be subject of a future paper. However, since in previous work on Davydov's method [2, 13] his incorrect derivation of equations of motion was used, it seems to be interesting in itself to study the dynamics of the system using correct equations.

3. Results and discussion

The equations of motion have been solved using a fourth-order Runge–Kutta method [18] and the dynamics were calculated over about 26 ps. We used as example the parameter set $W = 30\ \mathrm{N\ m^{-1}}$ and $X = 20$ pN at 300 K, where a travelling soliton is found and varied τ from 5 fs (sufficient for $T = 0$ K) to 0.3125 fs to 0.156 25 fs. The results did not change using the last two τ-values and the total energy is conserved in the region of 1–50 neV, the norm in the 1–50 ppb region. The small size of τ is necessary, because in the exponents of D_{nm} the time variation in b_{nk} is multiplied by v_k which for small frequencies is of the order 100. To be sure that the results are not simply numerical garbage due to the small τ-value or small denominators a_n, we compared the above-described calculation with that using double precision (128 bit per word) instead of the usual single precision (64 bit per word) through 10.5 ps. The results of both calculations are the same. As figure 1(a) shows for the above-mentioned example with $\tau = 0.3125$ fs the soliton disperses after reflection at the chain end. Thus we had to test whether this

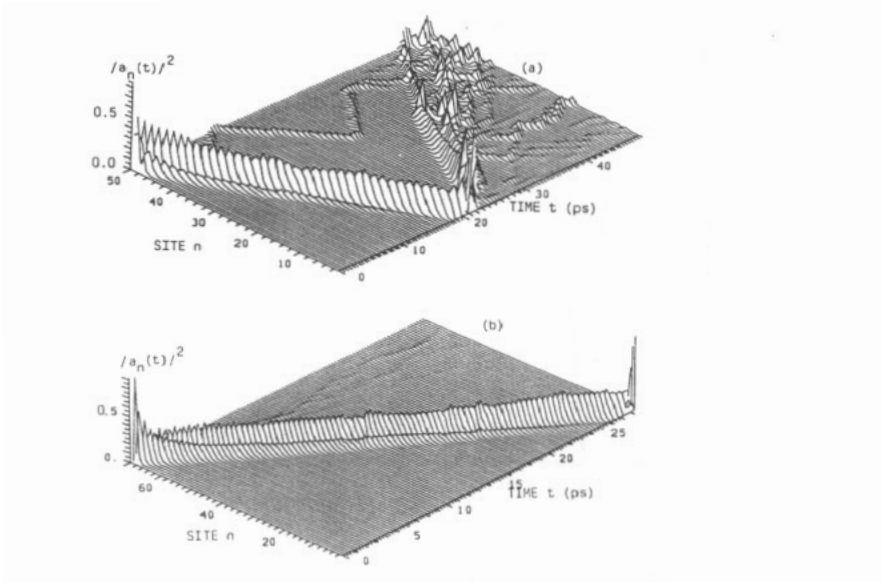

Figure 1. Time evolution of the probability to find an amide-I quantum $|a_n(t)|^2$ at site n (W = 30 N m^{-1}, X = 20 pN) at T = 300 K (τ = 0.3125 fs): (a) N = 50; (b) N = 70.

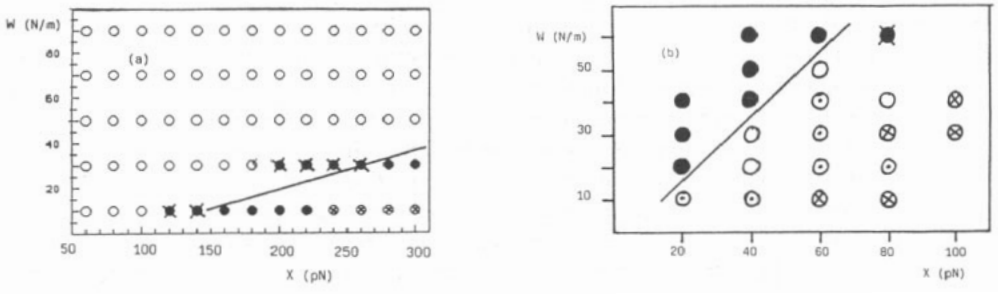

Figure 2. Survey of the (X, W) parameter for the $|D_1\rangle$ *ansatz* state: (a) T = 0 K, τ = 5 fs; (b) T = 300 K, τ = 0.156 25 fs. Each circle denotes a simulation (●, travelling soliton; ✖, travelling, slowly dispersive solitary wave; ⊗, pinned soliton; ○, dispersion after interaction with lattice sound reflected from the chain end; ⊙, pinned after interaction with lattice sound); all calculations over about 26 ps.

dispersion is only due to reflection at the free boundary or due to the lifetime of the soliton in the system. For this purpose we repeated the simulations using N = 60 and N = 70 units (figure 1(b)). Obviously the soliton is destroyed only at the chain end and can pass through much longer chains also.

We performed a survey of the (X, W) parameter space. The results are shown in figure 2, where each circle represents a simulation performed (7.8 h CPU time on a CDC Cyber 995E computer for each simulation at 300 K with τ = 0.156 25 fs). Obviously at T = 0 K, solitons occur at much larger values of X (figure 2(a)) and smaller values of W than at 300 K (figure 2(b)). The reason for that is the negative real part of the exponents in D_{nm} which increases in absolute value for increasing T. In turn these factors decrease

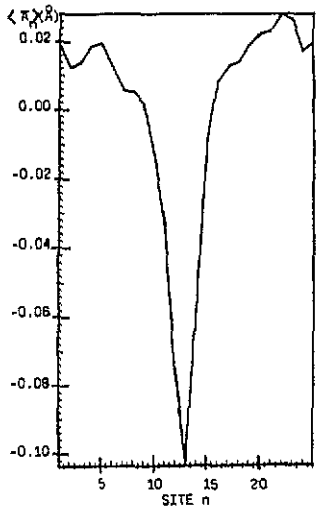

Figure 3. The averaged quantity $\langle A_n \rangle$ (see text) as function of site for $W = 13\ \mathrm{N\ m^{-1}}$, $X = 62$ pN, at $T = 50$ K.

effectively the dipole–dipole coupling J which is responsible for dispersion. In this way a larger temperature can stabilize solitons at smaller values of X. This is consistent with results reported by Cruzeiro *et al* [13], although the effect is far more pronounced in our case using the quantum mechanically correct equations of motion.

One may ask whether it is correct to introduce temperature in an averaged way as done here and, if not, whether fluctuations taken explicitly into account could destroy the solitons. However, we have shown in our previous work [11] that in case of the $|D_2\rangle$ *ansatz* models with explicit random fluctuations and our model using a lattice prepard to $T = 300$ K in a deterministic way lead to comparable results.Thus we are confident that in the $|D_1\rangle$ case the same conclusion holds. The other problem is the approximate nature of the $|D_1\rangle$ state. To improve the *ansatz* in this respect we plan to take two-phonon terms into accout in the generator of the unitary transformation [15]. However, it would be desirable to extend the exact quantum Monte Carlo simuations performed by Wang *et al* [19] for $W = 13\ \mathrm{N\ m^{-1}}$, $X = 62$ pN, to parameter values where we find travelling solitons to confirm our conclusions. It is difficult to compare simulations such as ours with the equilibrium calculations in [19]. However, we introduced the symmetric interaction and cyclic boundary conditions into our program and found no soliton at 7 and 11.2 K for the parameter values used in [19]. However, at 0.27 and 2.8 K where Wang *et al* reported coherent structures we found a clear dispersion of the initial excitation either. At 300 K we observe a ($N = 25$, $n_0 = 13$) highly localized structure which might bear some similarities to a small polaron because of the small effective value of JD_{nm}. To obtain a comparable plot we detected at each time step the site n with maximum excitation probability $|a_{n'}|^2$. Then we rotate the coordinate system such that $n' = 13$ after rotation. Then $A_n(t) = [q_{n+1}(t) - q_n(t)]|a_{n'}|^{-2}$ is computed and averaged over all time steps. In figure 3 we show this quantity ($\langle A_n \rangle$) for $T = 50$ K. Note that in our simulations the small polaron-like structures show up between 40 and 50 K. Obviously the curve is similar to those shown in [19]. The minimum $\langle A_{13} \rangle = -0.1$ Å is close to the infinite-temperature limit found in [19] of -0.095 Å.

Scott [20] argues that, in an α-helix, three coupled chains are present. In order to simulate three chains with a one-chain model, Scott emphasizes that larger values of W and M ($=342m_p$) should be used. We performed simulations at 300 K with the parameter

sets of Scott. However, it would probably be more reasonable to treat the three coupled chains explicitly. Work along this line is in progress. At $W = 39$ and $58.5\ \mathrm{N\ m^{-1}}$, $X = 35$ pN, we find a travelling soliton for roughly 10 ps. It disperses after interaction with the lattice sound. Thus in larger chains it might be able to survive for more than roughly 30 lattice sites. At the corresponding parameter values with $X = 62$ pN we find an irregularly moving soliton for the two values of W. In other preliminary calculations we found travelling solitons for $X = 20$ pN and $W = 50$ and $60\ \mathrm{N\ m^{-1}}$ but not below $W = 50\ \mathrm{N\ m^{-1}}$. Therefore the larger mass considerably influences the window of soliton formation.

4. Conclusion

Keeping all limitations in mind we conclude that Davydov solitons remain stable at $X = 40$–60 pN if $W > 50\ \mathrm{N\ m^{-1}}$ holds. This might well be the case in proteins since the value $W = 13\ \mathrm{N\ m^{-1}}$ usually quoted is from crystalline formamide [17] where free hydrogen-bonded molecules vibrate while in proteins a vibration of a hydrogen bond requires distortion of the covalently bound helical backbone. This should increase the effective value of W substantially compared with $13\ \mathrm{N\ m^{-1}}$.

Thus theoretically the existence of Davydov solitons seems to be quite probable in proteins at 300 K. However, a definitive answer to the question of the existence of Davydov solitons can only be given by experiment. For instance injection–detection experiments as proposed by Knox [21] would be highly desirable.

Acknowledgments

The financial support of the Deutsche Forschungsgemeinschaft (project Ot/56-2) and of the Fonds der chemischen Industrie is gratefully acknowledged.

Appendix

In our modified *ansatz* we use a lattice already prepared with a thermal phonon distribution $|T\rangle$ as we did in case of the classical $|D_2\rangle$ *ansatz* state [11] instead of starting from a thermally averaged Lagrangian:

$$|D_1, T\rangle = \sum_n a_n(t)\hat{a}_n^+ |0\rangle_e \hat{W}_n |T\rangle. \tag{A1}$$

Here $\hat{W}_n$ is a unitary displacement operator

$$\hat{W}_n = \exp(\hat{S}_n)$$

$$\hat{S}_n = \sum_k (b_{nk}\hat{b}_k^+ - b_{nk}^*\hat{b}_k). \tag{A2}$$

$|T\rangle$ is a coherent state with $|B_k|^2$ phonons in each normal mode k:

$$|T\rangle = \exp(\hat{T})\,|0\rangle_p$$
$$\hat{T} = \sum_k (B_k \hat{b}_k^\dagger - B_k^* \hat{b}_k). \tag{A3}$$

$|B_k|^2$ is computed according to Bose–Einstein statistics:

$$|B_k|^2 = 1/[\exp(\hbar\omega_k/k_B T) - 1] \equiv v_k^2. \tag{A4}$$

$|T_k\rangle$ is an exact solution of the time-dependent Schrödinger equation

$$i\hbar(\partial/\partial t)|T_k\rangle = \hbar\omega_k(\hat{b}_k^\dagger \hat{b}_k + \tfrac{1}{2})|T_k\rangle \tag{A5}$$

if

$$B_k(t) = |B_k|\exp(-i\omega_k t). \tag{A6}$$

Furthermore

$$\hat{U}_{nk}|T_k\rangle = \exp(\hat{S}_{nk})\exp(\hat{T}_k)|0\rangle_p = \exp(\tfrac{1}{2}[\hat{S}_{nk}, \hat{T}_k])\exp(\hat{S}_{nk} + \hat{T}_k)|0\rangle_p. \tag{A7}$$

With

$$[\hat{S}_{nk}, \hat{T}_k] = b_{nk}B_k^* - b_{nk}^* B_k \tag{A8}$$

we obtain our final *ansatz* state as

$$|D_1, T\rangle = \sum_n a_n(t)\hat{a}_n^\dagger |0\rangle_e \exp\left(\tfrac{1}{2}\sum_k (b_{nk}B_k^* - b_{nk}^* B_k)\right)$$
$$\times \exp\left(\sum_k (c_{nk}b_k^\dagger - c_{nk}^*\hat{b}_k)\right)|0\rangle_p \tag{A9}$$

where

$$c_{nk}(t) = b_{nk}(t) + v_k \exp(-i\omega_k t). \tag{A10}$$

Thus the phonon part consists of coherent states with amplitudes $c_{nk}(t)$, modulated by a phase factor. Then the Lagrangian is given by (see [15] for details of the method)

$$L = L_t - H + \frac{i\hbar}{2}\sum_{nk} |a_n|^2 v_k[(\dot{b}_{nk} + i\omega_k b_{nk})\exp(i\omega_k t)$$
$$- (\dot{b}_{nk}^* - i\omega_k b_{nk}^*)\exp(-i\omega_k t)] \tag{A11}$$

$$L_t = \frac{i\hbar}{2}\left\{\sum_n (\dot{a}_n a_n^* - \dot{a}_n^* a_n) + \sum_{nk} |a_n|^2(\dot{c}_{nk}c_{nk}^* - \dot{c}_{nk}^* c_{nk})\right\} \tag{A12}$$

$$H = \langle D_1, T|\hat{H}|D_1, T\rangle = \sum_n \Big((E_0 + E_n)|a_n|^2$$
$$- J_n a_n^* a_{n+1} D_{n,n+1} - J_{n-1}a_n^* a_{n-1} D_{n,n-1}$$
$$+ |a_n|^2 \sum_k \hbar\omega_k\{B_{nk}[b_{nk} + b_{nk}^* + 2v_k\cos(\omega_k t)]$$
$$+ |b_{nk}|^2 + v_k^2 + v_k[b_{nk}\exp(+i\omega_k t) + b_{nk}^*\exp(-i\omega_k t)]\}\Big) \tag{A13}$$

$$D_{nm} = \exp\Big(\sum_k [b^*_{nk}b_{mk} - \tfrac{1}{2}(|b_{nk}|^2 + |b_{mk}|^2) + (b^*_{nk} - b^*_{mk})v_k\, e^{-i\omega_k t} - (b_{nk} - b_{mk})v_k\, e^{i\omega_k t}]\Big). \tag{A14}$$

From this, equations of motion are obtained with the help of the Euler–Lagrange equations:

$$(d/dt)(\partial L/\partial \dot{a}_n) - \partial L/\partial a_n = 0$$
$$(d/dt)(\partial L/\partial \dot{b}_{nk}) - \partial L/\partial b_{nk} = 0. \tag{A15}$$

In [15] it is shown that for the $|D_1\rangle$ state the Euler–Lagrange method leads to the same equations of motion as projection techniques, time-dependent variation principle and Heisenberg operator equations, while Davydov's method [13] (treating $\langle D_1|\hat{H}|D_1\rangle$ as a classical Hamiltonian function) leads to different equations of motion, which do not even reproduce special analytically soluble cases ($J = 0$). The explicit form of the equations derived from (15) and our modified *ansatz* state as well as numerical applications will be published elsewhere.

References

[1] Davydov A S and Kislukha N I 1973 *Phys. Status Solidi* b **59** 465
Davydov A S 1979 *Phys. Scr.* **20** 387
[2] Davydov A S 1980 *Zh. Eksp. Teor. Fiz.* **78** 789 (Engl. Transl. 1980 *Sov. Phys.–JETP* **51** 397)
[3] Scott A C 1982 *Phys. Rev.* A **26** 57; 1984 *Phys. Scr.* **29** 279
MacNeil L and Scott A C 1984 *Phys. Scr.* **29** 284; *Phil. Trans. R. Soc.* A **315** 423
[4] Förner W and Ladik J 1991 *Davydov's Soliton Revisited (NATO Adv. Study Inst. Ser., Ser. B 243) ed P L Christiansen and A C Scott* (New York: Plenum)
[5] Halding J and Lomdahl P S 1987 *Phys. Lett.* A **124** 37
[6] Lomdahl P S and Kerr W C 1985 *Phys. Rev. Lett.* **55** 1235
[7] Lawrence A F, McDaniel J C, Chang D B, Pierce B M and Birge R R 1986 *Phys. Rev.* A **33** 1188
[8] Bolterauer H 1986 *Structure Coherence and Chaos, Proc. MIDIT 1986 Workshop* (Manchester: Manchester University Press)
[9] Cottingham J P and Schweitzer J W 1989 *Phys. Rev. Lett.* **62** 1792
[10] Motschmann H, Förner W and Ladik J 1989 *J. Phys.: Condens. Matter* **1** 5083
[11] Förner W 1991 *J. Phys.: Condens. Matter* **3** 4333
[12] Brown D W, Lindenberg K and West B J 1986 *Phys. Rev.* A **33** 4104, 4110; 1987 *Phys. Rev.* B **35** 6169; 1988 *Phys. Rev.* B **37** 2946
Brown D W 1988 *Phys. Rev.* A **37** 5010
[13] Cruzeiro L, Halding J, Christiansen P L, Skovgaard O and Scott A C 1988 *Phys. Rev.* A **37** 880
[14] Mechtly B and Shaw P B 1988 *Phys. Rev.* B **38** 3075
[15] Skrinjar M J, Kapor D V and Stojanovic S D 1988 *Phys. Rev.* A **38** 6402
[16] Förner W 1991 *Phys. Rev.* A **44** 2694
[17] Itoh K and Shimanouchi T 1972 *J. Mol. Spectrosc.* **42** 86
[18] Stiefel J 1965 *Einführung in die numerische Mathematik* (Stuttgart: Teubner)
[19] Wang X, Brown D W and Lindenberg K 1989 *Phys. Rev. Lett.* **62** 1796
[20] Scott A C *Conf. on Nonlinear Sciences: The Next Decade (Los Alamos National Laboratory, 21 May, 1990)*
[21] Knox R S 1991 *Davydov's Soliton Revisited* (NATO Adv. Study Inst. Ser., Ser. B, 243) ed P L Christiansen and A C Scott (New York: Plenum)