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QUANTUM-MECHANICAL DERIVATION OF THE DAVYDOV EQUATIONS FOR MULTI-QUANTA STATES

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Davydov and Kislukha¹ suggested in the 1970's that nonlinear self-trapping could serve as a method of energy transport along quasi-one-dimensional chains of molecules. The problem was to explain how the energy released by hydrolysis of adenosine triphosphate and transferred to proteins in biological systems remains localized and moves along the protein chains at a reasonable rate to perform useful biological functions. The α -helix protein structure was considered, which consists of three chains of hydrogen-bonded peptide groups (HNCO) with associated side groups which contribute to the molecular mass but are assumed dynamically inert. The coupled fields which they suggested are relevant in this problem are a high frequency intramolecular vibration of the peptide groups (the Amide-I or C=O stretch mode, at about 1665 cm^{-1}), and the low frequency vibrations of the entire peptide groups (and associated side groups). These fields are coupled through the dependence of the Amide-I energy on the length of the hydrogen bond coupling neighboring peptide groups.² The Hamiltonian Davydov used to describe this situation is the same as that used for the polaron problem (the Froehlich Hamiltonian for electron-phonon interactions) with some changes in the meaning of the symbols. Davydov's method of analysis^{1,3} of this Hamiltonian led to connections with ideas of soliton propagation in other physical systems.⁴

Following Davydov's original suggestion, the model has been elaborated by Scott and collaborators to describe more accurately the three-chain structure of α -helix, and numerical calculations have been carried out which verify the existence of self-trapped states in this model.⁵

Our purpose here is to present a derivation of the Davydov equations which employs only quantum-mechanical techniques. The derivation here is more general than our previous treatment of this problem⁶ because we use an *Ansatz* which has

present several quanta of the high frequency oscillator system rather than just one quantum.⁷ Since some steps of the calculation that follows are the same as those in our paper⁶ which treats the single quantum case, reference will be made to that paper for some of the those details.

Davydov's Hamiltonian is^{1,3}

$$H = \sum_n \left[E_0 B_n^\dagger B_n - J (B_{n+1}^\dagger B_n + B_n^\dagger B_{n+1}) \right] \quad (1)$$

$$+ \sum_n \left[\frac{p_n^2}{2m} + \frac{1}{2} w (u_{n+1} - u_n)^2 \right] + \chi \sum_n (u_{n+1} - u_{n-1}) B_n^\dagger B_n$$

$$= H_v + H_p + H_{iv}.$$

Here, B_n^\dagger and B_n are boson creation and annihilation operators for quanta of intramolecular vibrations with energy $E_0 = 1665 \text{ cm}^{-1}$ at site n (the C=O stretch mode), u_n and p_n are the molecular displacement and momentum operators for the molecule at site n , m and w are the molecular mass and intermolecular force constant, and J is the intersite transfer energy produced by dipole-dipole interactions. The non-linear coupling constant χ arises from modulation of the on-site energy by the molecular displacements. The vibrational part H_v , the phonon part H_p , and the interaction part H_{iv} are defined to be the individual terms in (1).

The phonon part of the Hamiltonian can be cast into familiar form in terms of phonon creation and annihilation operators by the use of the standard transformation

$$u_n = \sum_q \left[\frac{\hbar}{2Nm\omega_q} \right]^{1/2} e^{iqnl} (a_{-q}^\dagger + a_q), \quad (2a)$$

$$p_n = \sum_q \left[\frac{m\hbar\omega_q}{2N} \right]^{1/2} e^{iqnl} i (a_{-q}^\dagger - a_q). \quad (2b)$$

In these formulas l is the lattice spacing (the distance between peptide groups), and

$$\omega_q = 2(w/m)^{1/2} |\sin(ql/2)| \quad (3)$$

is the dispersion relation for H_p .

To understand the dynamics arising from the Hamiltonian (1), we make the *Ansatz* for the state vector

$$|\psi(t)\rangle = \frac{1}{\sqrt{Q!}} \left[\sum_n a_n(t) B_n^\dagger \right]^Q \exp \left\{ -\frac{i}{\hbar} \sum_j \left[\beta_j(t) p_j - \pi_j(t) u_j \right] \right\} |0\rangle, \quad (4)$$

where $|0\rangle$ is the ground state vector (i.e. it is annihilated both by B_n and by the phonon operators a_q). Davydov's original *Ansatz*^{1,3} was the $Q = 1$ case of this formula. Assuming that the time evolution of this state vector is approximately the same as that of the (unknown) exact state vector, one can then understand the system behavior by finding the time evolution of the three sets of unknown functions $a_n(t)$, $\beta_n(t)$, and $\pi_n(t)$.

First, we establish the necessary conditions for this state vector to be normalized. The normalization is

$$\langle \psi(t) | \psi(t) \rangle = \frac{1}{Q!} \sum_{\substack{m_1 \dots m_Q \\ n_1 \dots n_Q}} a_{m_1}^* \dots a_{m_Q}^* a_{n_1} \dots a_{n_Q} \langle 0 | B_{m_1} \dots B_{m_Q} B_{n_1}^\dagger \dots B_{n_Q}^\dagger | 0 \rangle. \quad (5)$$

By using mathematical induction one can show that the ground state expectation value appearing in (5) is equal to the $Q \times Q$ permanent

$$\langle 0 | B_{m_1} \dots B_{m_Q} B_{n_1}^\dagger \dots B_{n_Q}^\dagger | 0 \rangle = \text{per}(\delta_{m_i n_j}); \quad i, j = 1, \dots, Q. \quad (6)$$

Here $\delta_{i,j}$ is the Kronecker delta. A permanent is evaluated similarly to a determinant except that all of the terms are taken with positive signs. When we substitute this permanent (6) of Kronecker deltas into (5), we find that (5) reduces to $Q!$ identical terms each of which has Q identical factors, so that

$$\langle \psi(t) | \psi(t) \rangle = \frac{1}{Q!} \sum_{m_1 \dots m_Q} |a_{m_1}|^2 \dots |a_{m_Q}|^2 Q! = \left(\sum_m |a_m|^2 \right)^Q. \quad (7)$$

Therefore a necessary and sufficient condition for the state vector to be normalized,

$$\langle \psi(t) | \psi(t) \rangle = 1, \quad (8)$$

is that the amplitudes satisfy

$$\sum_m |a_m|^2 = 1. \quad (9)$$

In order to derive the Davydov equations implied by the above *Ansatz*, we need to know the average number of quanta at any given site,

$$\langle N_p \rangle = \langle \psi(t) | B_p^\dagger B_p | \psi(t) \rangle. \quad (10)$$

From this we can subsequently determine the average total number of quanta present. We substitute (4) into (10) and then use the boson commutation relations to get

$$\begin{aligned} \langle N_p \rangle = & \frac{1}{Q!} \sum_{\substack{m_1 \dots m_Q \\ n_1 \dots n_Q}} a_{m_1}^* \dots a_{m_Q}^* a_{n_1} \dots a_{n_Q} \\ & \times \left\{ \langle 0 | B_{m_1} \dots B_{m_Q} B_p B_{n_1}^\dagger \dots B_{n_Q}^\dagger B_p^\dagger | 0 \rangle - \langle 0 | B_{m_1} \dots B_{m_Q} B_{n_1}^\dagger \dots B_{n_Q}^\dagger | 0 \rangle \right\} \end{aligned} \quad (11)$$

The two ground state expectation values in (11) are a $(Q+1) \times (Q+1)$ permanent and a $Q \times Q$ permanent, respectively. The evaluation of this quantity is explained in the appendix. The result is

$$\langle N_p \rangle = Q |a_p|^2, \quad (12)$$

which implies

$$\langle \sum_p N_p \rangle = Q \quad (13)$$

by (9).

The interpretations of $\beta_n(t)$ and $\pi_n(t)$ are obtained as follows. Davydov³ points out that the part of $|\psi(t)\rangle$ depending on the displacement and momentum operators is a coherent state of the normal mode creation and annihilation operators. A coherent

state for the mode with wavevector q is⁸

$$|\alpha_q\rangle = \exp(\alpha_q a_q^\dagger - \alpha_q^* a_q) |0\rangle. \quad (14)$$

To see that (4) is a coherent state of all the normal modes, we use (2) to show that

$$-\frac{i}{\hbar} \sum_n (\beta_n p_n - \pi_n u_n) = \sum_q (\alpha_q a_q^\dagger - \alpha_q^* a_q), \quad (15)$$

where

$$\alpha_q = \left[\frac{m \omega_q}{2\hbar} \right]^{1/2} \beta_q + i \left[\frac{1}{2m \hbar \omega_q} \right]^{1/2} \pi_q. \quad (16)$$

[Here β_q is the spatial Fourier transform of β_n ,

$$\beta_q = \frac{1}{\sqrt{N}} \sum_n e^{-iqn} \beta_n, \quad (17)$$

and similarly for π_q .] We substitute (15) into (4) and get a factor of the form (14) for every normal mode. With the property

$$\langle \alpha_q | a_q | \alpha_q \rangle = \alpha_q, \quad (18)$$

and also using (2), (16), and (17), we straightforwardly obtain

$$\langle \psi(t) | u_n | \psi(t) \rangle = \beta_n(t), \quad (19a)$$

$$\langle \psi(t) | p_n | \psi(t) \rangle = \pi_n(t). \quad (19b)$$

The basic assumption in deriving the equations of motion is that $|\psi(t)\rangle$ is a solution of the time-dependent Schroedinger equation

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = H |\psi(t)\rangle. \quad (20)$$

Since (19) identifies $\beta_n(t)$ and $\pi_n(t)$ as expectation values, standard quantum-mechanical procedure gives

$$\dot{\beta}_n(t) = \frac{1}{i\hbar} \langle \psi(t) | [u_n, H] | \psi(t) \rangle, \quad (21a)$$

$$i\dot{\pi}_n(t) = \frac{1}{i\hbar} \langle \psi(t) | [p_n, H] | \psi(t) \rangle. \quad (21b)$$

The commutators are

$$[u_n, H] = i\hbar p_n / m, \quad (22a)$$

$$[p_n, H] = i\hbar \omega (u_{n+1} - 2u_n + u_{n-1}) + i\hbar \chi (B_{n+1}^\dagger B_{n+1} - B_{n-1}^\dagger B_{n-1}). \quad (22b)$$

Using (10), (12) and (19), we get one of Davydov's equations

$$m \ddot{\beta}_n = \omega (\beta_{n+1} - 2\beta_n + \beta_{n-1}) + Q \chi (|a_{n+1}|^2 - |a_{n-1}|^2). \quad (23)$$

The presence of Q quanta for the vibron oscillators increases the driving force on the phonon field by that factor, compared with the one-quantum case.

Next we derive the equation for $a_n(t)$. First we introduce a notation for the two parts of the state vector in (4):

$$|\psi(t)\rangle = |Q,a\rangle |\beta,\pi\rangle; \quad (24)$$

[for economy of notation the site and time-dependence of $a_n(t)$, $\beta_n(t)$ and $\pi_n(t)$ are left implicit]. The left-hand-side of the Schroedinger equation (20) is

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = \left\{ i\hbar \frac{\partial}{\partial t} |Q,a\rangle \right\} |\beta,\pi\rangle + |Q,a\rangle \left\{ i\hbar \frac{\partial}{\partial t} |\beta,\pi\rangle \right\} \quad (25)$$

Since all the operators defining $|Q,a\rangle$ commute, it is straightforward to show that

$$i\hbar \frac{\partial}{\partial t} |Q,a\rangle = \sqrt{Q} \left[\sum_n i\hbar \dot{a}_n B_n^\dagger \right] |Q-1,a\rangle \quad (26)$$

The other time derivative appearing in (25) is evaluated in Ref. 6 (the coherent state lattice part of the wave function is the same in these two calculations).

$$i\hbar \frac{\partial}{\partial t} |\beta,\pi\rangle = \sum_n \left[\dot{\beta}_n p_n - \dot{\pi}_n u_n + \frac{1}{2} (\beta_n \dot{\pi}_n - \dot{\beta}_n \pi_n) \right] |\beta,\pi\rangle. \quad (27)$$

Taking the inner product of (26) and (27) with $\langle \beta,\pi |$ and using (19) gives the reduction to vibron operators of the left-hand-side of the Schroedinger equation.

$$\begin{aligned} i\hbar \langle \beta,\pi | i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle \\ = \sqrt{Q} \left[\sum_n i\hbar \dot{a}_n B_n^\dagger \right] |Q-1,a\rangle + |Q,a\rangle \frac{1}{2} \sum_n \left[\dot{\beta}_n \pi_n - \dot{\pi}_n \beta_n \right] \end{aligned} \quad (28)$$

Similarly, for the right-hand-side of the Schroedinger equation

$$\begin{aligned} \langle \beta,\pi | H_v + H_p + H_{im} |\psi(t)\rangle = H_v |Q,a\rangle + |Q,a\rangle W(t) \\ + \chi \sum_n (\beta_{n+1} - \beta_{n-1}) B_n^\dagger B_n |Q,a\rangle. \end{aligned} \quad (29)$$

The quantity $W(t)$ is the phonon energy; the evaluation of this quantity given in Ref. 6 also applies here.

$$W(t) = \langle \beta,\pi | H_p | \beta,\pi \rangle = \sum_n \left[\frac{1}{2m} \pi_n^2 + \frac{1}{2} w (\beta_{n+1} - \beta_n)^2 \right] + \sum_q \frac{1}{2} \hbar \omega_q \quad (30)$$

We combine (28) and (29) to get the reduction of the time-dependent Schroedinger equation to vibron operators.

$$\begin{aligned} \sqrt{Q} \left[i\hbar \sum_n \dot{a}_n B_n^\dagger \right] |Q-1,a\rangle = H_v |Q,a\rangle \\ + \chi \sum_n (\beta_{n+1} - \beta_{n-1}) B_n^\dagger B_n |Q,a\rangle + \left\{ W(t) - \frac{1}{2} \sum_n (\dot{\beta}_n \pi_n - \dot{\pi}_n \beta_n) \right\} |Q,a\rangle. \end{aligned} \quad (31)$$

Using (4) to write the state $|Q-1,a\rangle$ and renaming the summation variable n on the left-hand-side of (31) as n_Q , we get

$$\sqrt{Q} \left[i\hbar \sum_n \dot{a}_n B_n^\dagger \right] |Q-1,a\rangle = \frac{Q}{\sqrt{Q!}} \sum_{n_1, \dots, n_Q} a_{n_1} \dots a_{n_Q} (i\hbar \dot{a}_{n_Q}) B_{n_1}^\dagger \dots B_{n_Q}^\dagger |0\rangle. \quad (32)$$

The evaluation of the right-hand-side of (31) requires operating with H_v and H_{int} on the vibron state $|Q, a\rangle$. Both of these terms require application of two boson operators, for possibly different sites, to $|Q, a\rangle$. This evaluation is effected by using the following identity, which can be proved by mathematical induction.

$$\begin{aligned} & (B_{l_1}^\dagger B_{l_2}) B_{n_1}^\dagger \cdots B_{n_Q}^\dagger |0\rangle \\ &= (\delta_{l_2 n_1} B_{l_1}^\dagger B_{n_2}^\dagger \cdots B_{n_Q}^\dagger + \delta_{l_2 n_2} B_{n_1}^\dagger B_{l_1}^\dagger B_{n_3}^\dagger \cdots B_{n_Q}^\dagger + \cdots + \delta_{l_2 n_Q} B_{n_1}^\dagger \cdots B_{n_{Q-1}}^\dagger B_{l_1}^\dagger) |0\rangle. \end{aligned} \quad (33)$$

There are Q terms here, each with Q factors. With this formula, the terms involved in the application of H_v can be shown to be

$$\sum_l B_l^\dagger B_l |Q, a\rangle = \frac{Q}{\sqrt{Q!}} \sum_{n_1, \dots, n_Q} a_{n_1} \cdots a_{n_Q} B_{n_1}^\dagger \cdots B_{n_Q}^\dagger |0\rangle, \quad (34)$$

and

$$\begin{aligned} & \sum_l \left[B_l^\dagger B_{l+1} + B_{l+1}^\dagger B_l \right] |Q, a\rangle \\ &= \frac{Q}{\sqrt{Q!}} \sum_{n_1, \dots, n_Q} \left[a_{n_1} \cdots a_{n_{Q-1}} a_{n_Q+1} + a_{n_1} \cdots a_{n_{Q-1}} a_{n_Q-1} \right] B_{n_1}^\dagger \cdots B_{n_Q}^\dagger |0\rangle. \end{aligned} \quad (35)$$

The interaction term, also obtained by using (33), is

$$\begin{aligned} & \sum_l \left[\beta_{l+1} - \beta_{l-1} \right] B_l^\dagger B_l |Q, a\rangle \\ &= \frac{Q}{\sqrt{Q!}} \sum_{n_1, \dots, n_Q} \left[\beta_{n_Q+1} - \beta_{n_Q-1} \right] a_{n_1} \cdots a_{n_Q} B_{n_1}^\dagger \cdots B_{n_Q}^\dagger |0\rangle, \end{aligned} \quad (36)$$

We now insert (32), (34) and (36) into (31), equate coefficients of $B_{n_1}^\dagger \cdots B_{n_Q}^\dagger |0\rangle$ in every term, cancel common factors of a_{n_i} , and arrive at an equation for a_n .

$$\begin{aligned} i\hbar \dot{a}_n &= \left\{ E_0 + \frac{1}{Q} \left[W(t) - \frac{1}{2} \sum_m \left[\dot{\beta}_m \pi_m - \dot{\pi}_m \beta_m \right] \right] \right\} a_n \\ &\quad - J(a_{n+1} + a_{n-1}) + \chi(\beta_{n+1} - \beta_{n-1}) a_n. \end{aligned} \quad (37)$$

By making use of the equations of motion (23) for π_m and β_m and (30) for the phonon energy, we can rewrite the quantity in square brackets in (37) as

$$\begin{aligned} & \frac{1}{Q} \left[W(t) - \frac{1}{2} \sum_m \left[\dot{\beta}_m \pi_m - \dot{\pi}_m \beta_m \right] \right] \\ &= \frac{1}{Q} \sum_q \frac{1}{2} \hbar \omega_q + \frac{1}{2} \chi \sum_m \beta_m \left[|a_{m+1}|^2 - |a_{m-1}|^2 \right] \end{aligned} \quad (38)$$

The factor of Q^{-1} multiplying the zero-point energy is the only place that the equation for \dot{a}_n for the multi-quanta Davydov state differs from the corresponding equation for the single quantum case. It has been pointed out previously^{6,9} that some physically measurable quantities, e.g. optical spectra, are sensitive to this phase of $a_n(t)$. Therefore it is conceivable that such measurements might distinguish different values of Q .

We now perform a phase change on the amplitude a_n

$$a_n(t) \rightarrow a_n(t) \exp \left[-\frac{i}{\hbar} \int \chi(t') dt' \right], \quad (39)$$

where $\chi(t)$ is the site-independent terms in (37),

$$\chi(t) = E_0 + \frac{1}{Q} \sum_q \frac{1}{2} \hbar \omega_q + \frac{1}{2} \chi \sum_m \beta_m \left[|a_{m+1}|^2 - |a_{m-1}|^2 \right] \quad (40)$$

The equation of motion for the redefined a 's is

$$i \hbar \dot{a}_n = -J(a_{n+1} + a_{n-1}) + \chi(\beta_{n+1} - \beta_{n-1})a_n, \quad (41)$$

which is the other Davydov equation.

To summarize, the Davydov equations for the multi-quantum state (4) are equations (24) and (42). The multi-quantum property of the state results in a stronger driving force on the phonon modes (24) but *no* modification of the equation for the probability amplitudes.

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APPENDIX

The evaluation of the permanents appearing in (11) is explained here. The $(Q+1) \times (Q+1)$ permanent appearing first in that equation is

$$\text{per} \begin{bmatrix} \delta_{m_1 n_1} & \cdots & \delta_{m_1 n_Q} & \delta_{m_1 p} \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \delta_{m_Q n_1} & \cdots & \delta_{m_Q n_Q} & \delta_{m_Q p} \\ \delta_{p n_1} & \cdots & \delta_{p n_Q} & 1 \end{bmatrix} \quad (A1)$$

The element 1 in the lower right corner is δ_{pp} , which appears because two of the operators in (11) have the subscript p . The $Q \times Q$ permanent appearing second in (11) is the first Q rows and columns of this one.

When (A1) is expanded by the minors of the bottom row (with all positive signs because it is a permanent), the $Q \times Q$ minor of the element 1 is cancelled by the second permanent in (11). Thus the difference of the two permanents in (11) is the following sum of Q terms.

$$\begin{aligned}
 & \delta_{pn_1} \text{ per} \begin{bmatrix} \delta_{m_1 n_2} & \cdots & \delta_{m_1 p} \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \delta_{m_Q n_2} & \cdots & \delta_{m_Q p} \end{bmatrix} + \delta_{pn_2} \text{ per} \begin{bmatrix} \delta_{m_1 n_1} & \delta_{m_1 n_3} & \cdots & \delta_{m_1 p} \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \delta_{m_Q n_1} & \delta_{m_Q n_3} & \cdots & \delta_{m_Q p} \end{bmatrix} \\
 & + \cdots + \delta_{pn_Q} \text{ per} \begin{bmatrix} \delta_{m_1 n_1} & \cdots & \delta_{m_1 n_{Q-1}} & \delta_{m_1 p} \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \delta_{m_Q n_1} & \cdots & \delta_{m_Q n_{Q-1}} & \delta_{m_Q p} \end{bmatrix} \quad (A2)
 \end{aligned}$$

When we substitute this formula for the difference of the two permanents in (11) and use the Kronecker delta prefactors to replace the p subscripts in each permanent, all of these permanents become the same, and it is the same one as in (6), viz.

$$\text{per} \begin{bmatrix} \delta_{m_1 n_1} & \cdots & \delta_{m_1 n_Q} \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \delta_{m_Q n_1} & \cdots & \delta_{m_Q n_Q} \end{bmatrix} \equiv \text{per}(\delta_{m_i n_j}) \quad (A3)$$

Thus

$$\langle N_p \rangle = \frac{1}{Q!} \sum_{\substack{m_1 \cdots m_Q \\ n_1 \cdots n_Q}} a_{m_1}^* \cdots a_{m_Q}^* a_{n_1} \cdots a_{n_Q} \left[\delta_{pn_1} + \delta_{pn_2} + \cdots + \delta_{pn_Q} \right] \text{per}(\delta_{m_i n_j}). \quad (A4)$$

The permanent expands into $Q!$ terms in which every m_i is set equal to a different one of the n_j 's. This generates Q factors of $|a_{m_i}|^2$ in each of the $Q!$ terms. Then the Q Kronecker deltas in the square brackets give Q terms in each of which one of the n 's is set equal to p , and the other $Q-1$ are summed on, each giving the same result. The result is

$$\langle N_p \rangle = \frac{1}{Q!} |a_p|^2 Q Q! \left(\sum_n |a_n|^2 \right)^{Q-1} \quad (A5)$$

We use the normalization condition in (9) and obtain the result (12).

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