Exact analytic multi-quanta states of the Davydov Dimer

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Abstract

The Davydov model describes amide I energy transfer in proteins without dispersion or dissipation. In spite of five decades of study, there are few exact analytical results, especially for the discrete version of this model. Here we develop two methods to determine the exact orthonormal, multi-quanta, eigenstates of the Davydov dimer. The first method involves the integration of a system of ordinary differential equations and the second method applies purely algebraic
methods to this problem. We obtain the general expression of the eigenvalues for any number of quanta and also, as examples, apply the methods to the detailed derivation of the eigenvectors for one to four quanta, plus a brief example in the case of \( n = 5 \) and \( n = 6 \).

1 Introduction

The energy for most of the processes that keep cells alive comes from the chemical reaction of hydrolysis of adenosinetriphosphate (ATP). This chemical reaction is catalyzed by proteins and is used for processes like the transport of ions and other ligands across cell membranes, protein synthesis and folding, cell division, and many others. In spite of all the progress made about the molecular aspects of those processes, it is not yet known how the energy released in the hydrolysis of ATP is ultimately used for work. The basic assumption of the model due to the Ukrainian physicist Davydov [6, 7] is that, in proteins, the energy released is stored in the form of amide I vibrations which are essentially stretching vibrations of the C=O groups. Formally, the Davydov model is analogous to the polaron model in which a free electron attracts the positive crystal sites, leading to a local distortion which, in turn, lowers the energy of the electron. The electron and its associated lattice distortion then move in a correlated manner in crystal, constituting a so-called self-trapped state or polaron. In the Davydov model, the role of the electron is played by the amide I vibration, and its interaction with the lattice sites is due to the dependence of the amide I energy on the length of the hydrogen bond that connects the C=O groups. When the energy of the distortion of the hydrogen-bonded lattice is smaller than the reduction in the amide I energy, the amide I also becomes self-trapped, in a state known as the Davydov soliton [6, 7, 15, 14].

In the continuum approximation, it is possible to obtain analytical solutions for the amide I state and for the lattice distortion, in the form of localized sech pulses [6, 7, 11]. On the other hand, in the more realistic discrete version numerical simulations are the norm (see e.g. [15, 12, 11, 13, 14, 5, 2, 4, 8]). Here, our aim was to determine exact analytical eigenstates of the Davydov dimer.

The amount of energy released in the hydrolysis of ATP estimated from
The Hamiltonian for the Davydov dimer is

\[ H' = \epsilon'(a_1^\dagger a_1 + a_2^\dagger a_2) + J(a_1^\dagger a_2 + a_2^\dagger a_1) - \chi u(a_1^\dagger a_1 - a_2^\dagger a_2) + \frac{1}{2} k u^2 + \frac{1}{2 \mu} p^2, \]

where \( a_i^\dagger \) (\( a_i \)) are the boson creation (annihilation) operators for an amide I vibration in site \( i \), \( u \) is the displacement from the equilibrium value of the hydrogen bond between the two sites, \( p \) is the momentum associated with \( u \), \( \epsilon' \) is the energy of the amide I at zero displacement, \( J \) is the dipole-dipole interaction between amide I vibrations at neighbouring sites, \( \chi \) is the change in amide I energy with hydrogen-bond length, \( k \) is the elasticity of the hydrogen bond and \( \mu \) is the reduced mass of the two sites. While many authors consider the regime in which both the amide I and the hydrogen bond displacements are treated quantum mechanically, it has been shown that, in the thermal equilibrium regime, above 11 K its behaviour is indistinguishable from the mixed quantum-classical regime in which the displacements are treated classically [4]. Since we are concerned with events that take place at the (much higher) biological temperatures, in what follows the changes in hydrogen bond lengths shall be described as c-numbers. This constitutes the
mixed quantum-classical regime mentioned in the introduction.

Setting $\epsilon = \epsilon' k/\chi^2$, $V = Jk/\chi^2$, and $U = k/\chi u$ and neglecting the kinetic energy of the lattice (the last term in (1)) we get the following a-dimensional Hamiltonian $H = k/\chi^2 H'$:

$$H = \epsilon (a_1^\dagger a_1 + a_2^\dagger a_2) + V (a_1^\dagger a_2 + a_2^\dagger a_1) - U (a_1^\dagger a_1 - a_2^\dagger a_2) + \frac{1}{2} U^2$$

(2)

For the eigenstate calculations we ignore the first and last terms which merely shift the eigenenergies. I.e., the eigenstates depend only on $V$ and $U$.

3 Theory

To write the wavefunction we use a site-based basis set. Applying standard Dirac notation [16], for the dimer we write interchangeably

$$|\psi(n_i, n_j)\rangle = |n_i\rangle_1 |n_j\rangle_2$$

for a state with $n_i$ bosons on site 1 and $n_j$ bosons on site 2. Note that our basis states are orthonormal

$$k\langle n_i |n_j \rangle_\ell = \delta_{i,j} \delta_{k,\ell}.$$

With $n$ quanta we have a basis set with $N = n + 1$ elements

$$|\psi(n,0)\rangle, |\psi(n-1,1)\rangle, |\psi(n-2,2)\rangle, \ldots, |\psi(0,n)\rangle.$$

3.1 Eigenstates for $n=1$

Let us first consider the case $n = 1$, in which there is only one amide I excitation in the dimer. In this case there are two basis functions, namely, $|\psi_1\rangle = |\psi(1,0)\rangle$, representing the state in which the amide I excitation is in site 1 and $|\psi_2\rangle = |\psi(0,1)\rangle$, representing the state in which the amide I excitation is in site 2. Other choices are possible, provided we have a complete set, and it is simplest to choose an orthonormal set. The matrix $H$ that we
end up with (see below) depends on this choice. With the basis set we have chosen, we have:

\[ H |\psi_1\rangle = V |\psi_2\rangle - U |\psi_1\rangle , \]

and

\[ H |\psi_2\rangle = V |\psi_1\rangle + U |\psi_2\rangle , \]

so the matrix \( \mathbf{H} \) is

\[ \mathbf{H} = \langle \psi_i | H | \psi_j \rangle = \begin{bmatrix} -U & V \\ V & +U \end{bmatrix} . \]

The eigenvalues are \( E = \pm \sqrt{(U^2 + V^2)} \).

Since the eigenvalues are expressed in terms of \( \sqrt{(U^2 + V^2)} \), also for \( n > 1 \), it makes sense to parameterize \( U, V \) as \( U = -R \cos(\theta), V = R \sin(\theta) \). With this change the eigenvalues are \( E = \pm R \), and the eigenvectors are simple functions of \( \cos(\theta) \) and \( \sin(\theta) \). We will keep this parameterization in all that follows. We now have

\[ \mathbf{H} = R \sin(\theta) (a_1^\dagger a_2 + a_2^\dagger a_1) + R \cos(\theta) (a_1^\dagger a_1 - a_2^\dagger a_2) , \]

and

\[ \mathbf{H} = \langle \psi_i | H | \psi_j \rangle = \begin{bmatrix} R \cos(\theta) & R \sin(\theta) \\ R \sin(\theta) & -R \cos(\theta) \end{bmatrix} . \]

A simple calculation gives the eigenvalues of \( \mathbf{H} \) as \( E = \pm R \), as expected.

In the matrix \( \mathbf{H} \), \( R \) is an overall multiplicative constant, which affects the eigenvalues but not the eigenvectors. So, for all values of \( n \), we will switch to a modified Hamiltonian with \( R = 1 \). For \( n = 1 \) we get:

\[ \mathbf{H} = \begin{bmatrix} \cos(\theta) & \sin(\theta) \\ \sin(\theta) & -\cos(\theta) \end{bmatrix} . \tag{3} \]

Given the eigenvalues of this new Hamiltonian, we can recover the eigenvalues of the original Hamiltonian (2) by multiplying by \( R \) and adding \( n \epsilon + \frac{1}{2} U^2 \).

In the following calculations we will be interested in increasing values of \( n \), so it is worth a short discussion of the eigenvectors of \( \mathbf{H} \) even in this trivial case. Eigenvectors are only unique up to a constant multiplying factor, and the algebraic manipulation system Maple gives the eigenvectors of \( \mathbf{H} \) (3), as

\[ \left[ -\frac{\sin(\theta)}{\cos(\theta) + 1}, 1 \right]' \]
which become
\[ [\sin(\theta), \pm 1 - \cos(\theta)]' \]
on multiplication by the denominators.

3.2 Eigenstates for all values of \( n \)

We wish to determine the analytical expressions for the eigenvalues and eigen-vectors of the matrix \( H \) and of its generalizations to higher amide I quantum numbers, \( n > 1 \). To that end, we make use of the Lie Algebra, \( \mathfrak{sl}_2(\mathbb{C}) \). This is a complex, three dimensional vector space with basis \( \{\mathbf{e}, \mathbf{f}, \mathbf{h}\} \) and a \( \mathbb{C} \)-linear multiplication, \( * \), given by

\[
\mathbf{h} * \mathbf{e} = 2\mathbf{e}, \quad \mathbf{h} * \mathbf{f} = -2\mathbf{f}, \quad \mathbf{e} * \mathbf{f} = \mathbf{h}.
\]

There are representations of this algebra in which the roles of the basis elements are played by \( N \times N \) complex matrices, and the role of the multiplication operation by matrix commutation, for example:

\[
\mathbf{e} * \mathbf{f} = [\mathbf{e}, \mathbf{f}] = \mathbf{e}\mathbf{f} - \mathbf{f}\mathbf{e},
\]

etc.; the algebraic operations on the right hand side being straightforward matrix multiplication and addition.

The \( N \times N \) matrix representations of \( \mathfrak{sl}_2(\mathbb{C}) \) are not unique but one “standard” representation is:

\[
\mathbf{h} = \sum_{i=1}^{N} (N - 2i + 1) \mathbf{E}_{i,i} \quad (5)
\]
\[
\mathbf{e} = \sum_{i=1}^{N-1} \sqrt{i(N-i)} \mathbf{E}_{i,i+1} \quad (6)
\]
\[
\mathbf{f} = \sum_{j=1}^{N-1} \sqrt{j(N-j)} \mathbf{E}_{j+1,j} \quad (7)
\]

\( \mathbf{E}_{i,j} \) being the \( N \times N \) matrix with unity in the \( (i,j) \)th entry and zero elsewhere. Note, in particular, that \( \mathbf{h} \) is a diagonal matrix with entries \( \{N-1, N-3, \ldots, -N+3, -N+1\} \).
As shown in section\footnote{4} the $H$ matrices of interest to us are all of the form
\[ H(\theta) = \cos \theta \mathbf{h} + \sin \theta (\mathbf{e} + \mathbf{f}) \tag{8} \]
with $N = n+1$ and we wish to show that, in the first instance, the eigenvalues of $H$ are constant.

It is easy to see that
\[
\frac{\partial H(\theta)}{\partial \theta} = -\sin \theta \mathbf{h} + \cos \theta (\mathbf{e} + \mathbf{f})
\]
\[ = \frac{1}{2}(\mathbf{f} - \mathbf{e}) \ast H
\]
\[ = [\mathbf{p}, H].
\]
where $\mathbf{p} = \frac{1}{2}(\mathbf{f} - \mathbf{e})$ is a constant matrix.

If we write $P(\theta) = \exp (\mathbf{p} \theta)$ then
\[ H(\theta) = P(\theta)H(0)P^{-1}(\theta)
\]
\[ = P(\theta)\mathbf{h}P^{-1}(\theta)
\]
\[ \text{since } H(0) = \mathbf{h}. \]
Thus, the eigenvalues of $H(\theta)$ are the same as those of $\mathbf{h}$, namely, they are its diagonal entries, \{-N + 1, -N + 3, \ldots, N - 3, N - 1\}. This proves that, in terms of the number $n$ of amide I excitation, the energies of each eigenstate are simply given by:
\[ E_j = jR + n \epsilon + \frac{1}{2} U^2, \quad \text{for } j \text{ in } \{-n, -(n - 2), \ldots, (n - 2), n\}. \tag{9} \]

The corresponding eigenvectors, $V$, of $H(\theta)$ are related to $v$, the eigenvectors of $\mathbf{h}$, by
\[ V = P(\theta)v.
\]
where the $v$'s are simply the standard basis for $\mathbb{C}^N$.

We can construct the $V$'s by converting the above equation into a set of linear ordinary differential equations and solving with appropriate initial conditions. Thus let $v$ for $i = 1, 2, \ldots, N = n+1$ be the standard basis for $\mathbb{C}^N$. We solve the linear system
\[ \frac{\partial V}{\partial \theta} = \mathbf{p}V \tag{10} \]
with initial condition $V(0)^{(i)} = v^{(i)}$ for each $i$. Since $\mathbf{e}^T = \mathbf{f}$, we have $\mathbf{p}^T = -\mathbf{p}$ and hence $P(\theta)^TP(\theta) = \text{Id}$. So, $P(\theta)$ is a real unitary operator and if we
choose \( V(0)^{(i)} \) to be normalized to unity, \( V(\theta)^{(i)} \) will be unit vectors also. If \( V(0) \) is real, then the solution will be real also. In section 4, examples of using eq. (10) to determine exact normalized eigenvectors are presented. On the other hand, below we develop another, purely algebraic procedure for the same purpose.

The solutions to these equations belong to the span of a finite dimensional function space which we can describe if we know the eigenvalues of \( p \); that is, if we could diagonalize \( p \) as a matrix with entries \( \mu_i \) for \( i = 1, \ldots, n \), then the functions \( \exp \mu_i \theta \) will be a basis for the solution space. In fact it is not difficult to enlist the Lie representation theory again here. A complex representation of \( \mathfrak{sl}_2(\mathbb{C}) \), in which \( p \) spans the Cartan subalgebra, is given by the basis elements,

\[
\tilde{e} = \frac{1}{2}(h + i(e + f)), \quad h = i(f - e);
\]

(11) \hspace{1cm} (13)

that is, we have the commutation relations:

\[
[h, \tilde{e}] = 2\tilde{e}, \quad [h, \tilde{f}] = -2\tilde{f}, \quad [\tilde{e}, \tilde{f}] = 2h.
\]

Note that \( \tilde{h} = 2i\mathbf{p} \).

Since \( h \) acts diagonally on its eigenvectors, we seek a highest weight eigenvector, \( \tilde{v} \), such that [9]:

\[
\tilde{h}(\tilde{v}) = \tilde{\lambda}\tilde{v}, \quad \tilde{e}(\tilde{v}) = 0.
\]

(14)

By the general representation theory [2] it will be enough to show that \( \tilde{\lambda} = n \). The other eigenvalues will then, by necessity, be \( n - 2, n - 4, \ldots, -n \).

Equation (14) implies

\[
(h + 2if)\tilde{v} = \tilde{\lambda}\tilde{v}, \quad (h - 2ie)\tilde{v} = -\tilde{\lambda}\tilde{v},
\]

(15) \hspace{1cm} (16)

and each of these equations is respectively lower and upper triangular, so, in particular, the eigenvalues of \( h + 2if \) are exactly the eigenvalues of \( h \).
Given the standard form of $h$ with $h_{11} = n$ we have an inductive argument: if $\tilde{v}_1 \neq 0$ then $\tilde{\lambda} = n$; if $\tilde{v}_1 = 0$ then $\tilde{v}_2 = 0$ and so on.

Hence $\tilde{h}$ has eigenvalues $\{n, n-2, \ldots, -n\}$ and $p = -\frac{i}{2} \tilde{h}$ has eigenvalues

$$\left\{ \frac{i}{2} n, \frac{i}{2} (n-2), \ldots, -\frac{i}{2} n \right\}.$$

Our alternative construction of the eigenvectors can be made by identifying $\theta$-dependent raising and lowering operators, defined below as $f(\theta)$ and $e(\theta)$, respectively. The corresponding eigenvectors of $p$, $u^j$ for $j = 1, \ldots, N$, can be calculated by applying powers of $\tilde{f}$ to $\tilde{v}$. These are now complex valued eigenvectors. The eigenvalue of $u^j$ is $\mu_j = -i(N - 2j + 1)/2$.

To solve the problem we need only express $v^1 = (1, 0, \ldots, 0)$ as a linear sum of the $u^j$, with complex coefficients:

$$v^1 = \sum_{j=1}^{d} c_j u^j,$$

then

$$V^1 = \sum_{j=1}^{d} c_j \exp(p\theta) u^j$$

$$= \sum_{j=1}^{d} c_j \exp(\mu_j \theta) u^j.$$

This will be a real, unit vector.

To construct $V^2$, etc. note that we have raising and lowering operators:

$$e(\theta) = \exp(p\theta) e \exp(-p\theta)$$

$$= \sum_{k=0}^{\infty} \frac{\theta^k}{k!} \text{ad}_p^k e$$

$$f(\theta) = \exp(p\theta) f \exp(-p\theta)$$

$$= \sum_{k=0}^{\infty} \frac{\theta^k}{k!} \text{ad}_p^k f$$

for which we can obtain exact, finite expressions since

$$\text{ad}_p e = \frac{1}{2} [f - e, e] = -\frac{1}{2} h.$$
\[ \text{ad}_p e = -\frac{1}{4}[f - e, h] = -\frac{1}{2}(f + e), \]
\[ \text{ad}_p e = -\frac{1}{4}[f - e, f + e] = \frac{1}{2}h, \]

etc. That is,
\[ e(\theta) = -\frac{1}{2} \sin \theta h + \frac{1}{2}(1 + \cos \theta)e - \frac{1}{2}(1 - \cos \theta)f, \]
and, similarly,
\[ f(\theta) = -\frac{1}{2} \sin \theta h + \frac{1}{2}(1 + \cos \theta)f - \frac{1}{2}(1 - \cos \theta)e. \]

Note the eigenvectors are functions of half-angles when \( n \) is even and integral angles when \( n \) is odd because \( f(\theta) \) is a function of \( \cos \theta \) and \( \sin \theta \) applied to half-angle functions and integral angle functions in each case.

Now \( f(\theta) \) applied to \( V^1 \) gives \( V^2 \) and so on but the normalization will not be preserved. To fix this we need to divide by a factor of \( \sqrt{j(N-j)} \) when applying \( f(\theta) \) to \( V^j \).

We will illustrate this approach below in addition to the method solving (5-10).

4 Applications of Lie theory to multi-quanta states

Let us now see how (5-10) can be used to determine the multi-quanta eigenstates of the Davydov dimer.

n=1 Case

Starting with \( n = 1 \), the matrices \( h, f, e, \) and \( p \) are:
\[ h = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \quad f = \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}, \quad e = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}, \quad p = \begin{bmatrix} 0 & -\frac{1}{2} \\ \frac{1}{2} & 0 \end{bmatrix}. \]

and the ODEs (10) for the components of eigenvectors are:
\[ \frac{d}{d\theta} V_1(\theta) = -\frac{1}{2} V_2(\theta) \]
\[ \frac{d}{d\theta} V_2(\theta) = \frac{1}{2} V_1(\theta) \]
with general solution

\[
V_1(\theta) = C_1 \sin\left(\frac{1}{2}\theta\right) + C_2 \cos\left(\frac{1}{2}\theta\right),
\]

\[
V_2(\theta) = -C_1 \cos\left(\frac{1}{2}\theta\right) + C_2 \sin\left(\frac{1}{2}\theta\right).
\]

For the \(E_{-1} = -1\) eigenvalue, we have \(V_1(0) = 0, V_2(0) = 1\) and hence

\[C_1 = -1, \quad C_2 = 0,\]

giving the eigenvector

\[
\begin{bmatrix}
\sin\left(\frac{1}{2}\theta\right) \\ -\cos\left(\frac{1}{2}\theta\right)
\end{bmatrix}.
\]

which reduces to the normalized form of (4) after trigometric substitutions.

In the \(E = 1\) case, we have \(V_1(0) = 1, V_2(0) = 0\) and hence

\[C_1 = 0, \quad C_2 = 1,\]

giving

\[
\begin{bmatrix}
\cos\left(\frac{1}{2}\theta\right) \\ \sin\left(\frac{1}{2}\theta\right)
\end{bmatrix}.
\]

orthogonal to the above and again a normalized form of (4).

\[n = 2 \text{ Case}\]

We have

\[
H = \begin{bmatrix}
-2 \cos(\theta) & \sqrt{2}\sin(\theta) & 0 \\
\sqrt{2}\sin(\theta) & 0 & \sqrt{2}\cos(\theta) \\
0 & \sqrt{2}\sin(\theta) & 2\cos(\theta)
\end{bmatrix}.
\]

In the Lie theory we have

\[
h = \begin{bmatrix}
2 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & -2
\end{bmatrix}, \quad f = \begin{bmatrix}
0 & 0 & 0 \\
\sqrt{2} & 0 & 0 \\
0 & \sqrt{2} & 0
\end{bmatrix},
\]

\[
e = \begin{bmatrix}
0 & \sqrt{2} & 0 \\
0 & 0 & \sqrt{2} \\
0 & 0 & 0
\end{bmatrix}, \quad p = \begin{bmatrix}
0 & -\frac{1}{\sqrt{2}} & 0 \\
\frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} \\
0 & \frac{1}{\sqrt{2}} & 0
\end{bmatrix}.
\]
The ODEs for components of eigenvectors are
\[
\begin{align*}
\frac{d}{d\theta} V_1(\theta) &= -\frac{1}{\sqrt{2}} V_2(\theta) \\
\frac{d}{d\theta} V_2(\theta) &= \frac{1}{\sqrt{2}} V_1(\theta) - \frac{1}{\sqrt{2}} V_3(\theta) \\
\frac{d}{d\theta} V_3(\theta) &= \frac{1}{\sqrt{2}} V_2(\theta)
\end{align*}
\]
with general solution
\[
\begin{align*}
V_1(\theta) &= -\frac{1}{\sqrt{2}} \sin(\theta) C_3 + \frac{1}{\sqrt{2}} \cos(\theta) C_2 + C_1, \\
V_2(\theta) &= C_2 \sin(\theta) + C_3 \cos(\theta), \\
V_3(\theta) &= \frac{1}{\sqrt{2}} \sin(\theta) C_3 - \frac{1}{\sqrt{2}} \cos(\theta) C_2 + C_1.
\end{align*}
\]
For the \( E = -2, 0, +2 \) eigenvalues, we find in turn
\[
\begin{align*}
C_1 &= \frac{1}{2}, C_2 = \frac{1}{\sqrt{2}}, C_3 = 0, \\
C_1 &= 0, C_2 = 0, C_3 = 1, \\
C_1 &= \frac{1}{2}, C_2 = -\frac{1}{\sqrt{2}}, C_3 = 0.
\end{align*}
\]

\( n = 3 \) Case

We have
\[
H = \begin{bmatrix}
-3 \cos(\theta) & \sin(\theta) \sqrt{3} & 0 & 0 \\
\sin(\theta) \sqrt{3} & -\cos(\theta) & 2 \sin(\theta) & 0 \\
0 & 2 \sin(\theta) & \cos(\theta) & \sin(\theta) \sqrt{3} \\
0 & 0 & \sin(\theta) \sqrt{3} & 3 \cos(\theta)
\end{bmatrix}
\]
with eigenvalues \( E = -3, -1, +1, +3 \).

In the Lie theory we have
\[
\begin{align*}
h &= \begin{bmatrix}
3 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & -1 & 0 \\
0 & 0 & 0 & -3
\end{bmatrix},
\quad e = \begin{bmatrix}
0 & \sqrt{3} & 0 & 0 \\
0 & 0 & 2 & 0 \\
0 & 0 & 0 & \sqrt{3} \\
0 & 0 & 0 & 0
\end{bmatrix}, \\
f &= \begin{bmatrix}
0 & 0 & 0 & 0 \\
\sqrt{3} & 0 & 0 & 0 \\
0 & 2 & 0 & 0 \\
0 & 0 & \sqrt{3} & 0
\end{bmatrix},
\quad p = \begin{bmatrix}
0 & -\frac{1}{2} \sqrt{3} & 0 & 0 \\
\frac{1}{2} \sqrt{3} & 0 & -1 & 0 \\
0 & 1 & 0 & \frac{1}{2} \sqrt{3} \\
0 & 0 & \frac{1}{2} \sqrt{3} & 0
\end{bmatrix}.
\end{align*}
\]
\[
\begin{align*}
\frac{d}{d\theta} V_1(\theta) &= -\frac{1}{2}\sqrt{3} V_2(\theta), \\
\frac{d}{d\theta} V_2(\theta) &= \frac{1}{2}\sqrt{3} V_1(\theta) - V_3(\theta), \\
\frac{d}{d\theta} V_3(\theta) &= V_2(\theta) - \frac{1}{2}\sqrt{3} V_4(\theta), \\
\frac{d}{d\theta} V_4(\theta) &= \frac{1}{2}\sqrt{3} V_3(\theta).
\end{align*}
\]

with solution

\[
\begin{align*}
V_1(\theta) &= C_1 \sin \left(\frac{3}{2} \theta\right) + C_2 \cos \left(\frac{3}{2} \theta\right) + C_3 \sin \left(\frac{1}{2} \theta\right) + C_4 \cos \left(\frac{1}{2} \theta\right), \\
V_2(\theta) &= -\frac{1}{\sqrt{3}} \left(3C_1 \cos \left(\frac{3}{2} \theta\right) - 3C_2 \sin \left(\frac{3}{2} \theta\right) + C_3 \cos \left(\frac{1}{2} \theta\right) - C_4 \sin \left(\frac{1}{2} \theta\right)\right), \\
V_3(\theta) &= -\frac{1}{\sqrt{3}} \left(3C_2 \cos \left(\frac{3}{2} \theta\right) + 3C_1 \sin \left(\frac{3}{2} \theta\right) - C_4 \cos \left(\frac{1}{2} \theta\right) - C_3 \sin \left(\frac{1}{2} \theta\right)\right), \\
V_4(\theta) &= C_1 \cos \left(\frac{3}{2} \theta\right) - C_2 \sin \left(\frac{3}{2} \theta\right) - C_3 \cos \left(\frac{1}{2} \theta\right) + C_4 \sin \left(\frac{1}{2} \theta\right).
\end{align*}
\]

For the eigenvalues \(E_i\) we have sequentially

\[
\begin{align*}
C_1 &= 0, C_2 = \frac{3}{4}, C_3 = 0, C_4 = \frac{1}{4}, \\
C_1 &= -\frac{\sqrt{3}}{4}, C_2 = 0, C_3 = -\frac{\sqrt{3}}{4}, C_4 = 0, \\
C_1 &= 0, C_2 = \frac{\sqrt{3}}{4}, C_3 = 0, C_4 = -\frac{\sqrt{3}}{4}, \\
C_1 &= -\frac{3}{4}, C_2 = 0, C_3 = \frac{1}{4}, C_4 = 0,
\end{align*}
\]

giving the eigenvectors

\[
\begin{align*}
\begin{bmatrix}
\frac{3}{4} \cos \left(\frac{\theta}{2}\right) + \frac{1}{4} \cos \left(\frac{3\theta}{2}\right) \\
\frac{\sqrt{3}}{4} \left(\sin \left(\frac{\theta}{2}\right) + \sin \left(\frac{3\theta}{2}\right)\right) \\
\frac{3}{4} \sin \left(\frac{\theta}{2}\right) - \frac{1}{4} \sin \left(\frac{3\theta}{2}\right)
\end{bmatrix}, \\
\begin{bmatrix}
-\frac{\sqrt{3}}{4} \left(\sin \left(\frac{\theta}{2}\right) + \sin \left(\frac{3\theta}{2}\right)\right) \\
\frac{1}{4} \cos \left(\frac{\theta}{2}\right) + \frac{3}{4} \cos \left(\frac{3\theta}{2}\right) \\
-\frac{1}{4} \sin \left(\frac{\theta}{2}\right) + \frac{3}{4} \sin \left(\frac{3\theta}{2}\right)
\end{bmatrix}, \\
\begin{bmatrix}
\frac{\sqrt{3}}{4} \left(\cos \left(\frac{\theta}{2}\right) - \cos \left(\frac{3\theta}{2}\right)\right) \\
\frac{1}{4} \sin \left(\frac{\theta}{2}\right) - \frac{3}{4} \sin \left(\frac{3\theta}{2}\right) \\
\frac{\sqrt{3}}{4} \left(\cos \left(\frac{\theta}{2}\right) + \cos \left(\frac{3\theta}{2}\right)\right)
\end{bmatrix}, \\
\begin{bmatrix}
\frac{3}{4} \sin \left(\frac{\theta}{2}\right) + \frac{1}{4} \sin \left(\frac{3\theta}{2}\right) \\
\frac{\sqrt{3}}{4} \left(\cos \left(\frac{\theta}{2}\right) - \cos \left(\frac{3\theta}{2}\right)\right) \\
-\frac{\sqrt{3}}{4} \left(\sin \left(\frac{\theta}{2}\right) + \sin \left(\frac{3\theta}{2}\right)\right)
\end{bmatrix}.
\end{align*}
\]

Note that the elements of these are now \textit{linear} in \(\sin\) and \(\cos\) of \(\frac{\theta}{2}\) and \(\frac{3\theta}{2}\).
\( n = 4 \) Case

\[
H = \begin{bmatrix}
4 \cos(\theta) & 2 \sin(\theta) & 0 & 0 & 0 \\
2 \sin(\theta) & 2 \cos(\theta) & \sin(\theta) \sqrt{6} & 0 & 0 \\
0 & \sin(\theta) \sqrt{6} & 0 & \sin(\theta) \sqrt{6} & 0 \\
0 & 0 & \sin(\theta) \sqrt{6} & -2 \cos(\theta) & 2 \sin(\theta) \\
0 & 0 & 0 & 2 \sin(\theta) & -4 \cos(\theta)
\end{bmatrix}
\]

with eigenvalues \( E = -4, -2, 0, 2, 4 \).

In the Lie theory we have

\[
h = \begin{bmatrix}
4 & 0 & 0 & 0 & 0 \\
0 & 2 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & -2 & 0 \\
0 & 0 & 0 & 0 & -4
\end{bmatrix}, \quad e = \begin{bmatrix}
0 & 2 & 0 & 0 & 0 \\
0 & 0 & \sqrt{6} & 0 & 0 \\
0 & 0 & 0 & 0 & 2 \\
0 & 0 & 0 & 0 & 0
\end{bmatrix},
\]

\[
f = \begin{bmatrix}
0 & 0 & 0 & 0 & 0 \\
2 & 0 & 0 & 0 & 0 \\
0 & \sqrt{6} & 0 & 0 & 0 \\
0 & 0 & \sqrt{6} & 0 & 0 \\
0 & 0 & 0 & 2 & 0
\end{bmatrix}, \quad p = \begin{bmatrix}
0 & -1 & 0 & 0 & 0 \\
1 & 0 & -\frac{\sqrt{6}}{2} & 0 & 0 \\
0 & \frac{\sqrt{6}}{2} & 0 & -\frac{\sqrt{6}}{2} & 0 \\
0 & 0 & \frac{\sqrt{6}}{2} & 0 & 1 \\
0 & 0 & 0 & 1 & 0
\end{bmatrix}
\]

\[
\frac{d}{d\theta} V_1(\theta) = -V_2(\theta),
\]

\[
\frac{d}{d\theta} V_2(\theta) = V_1(\theta) - \sqrt{\frac{2}{3}} V_3(\theta),
\]

\[
\frac{d}{d\theta} V_3(\theta) = \sqrt{\frac{2}{3}} V_2(\theta) - \sqrt{\frac{2}{3}} V_4(\theta),
\]

\[
\frac{d}{d\theta} V_4(\theta) = \frac{1}{2} \sqrt{3} V_3(\theta) - V_5(\theta),
\]

\[
\frac{d}{d\theta} V_5(\theta) = V_4(\theta).
\]

general solution is

\[
V_1(\theta) = C_1 + C_2 \sin(2\theta) + C_3 \cos(2\theta) + C_4 \sin(\theta) + C_5 \cos(\theta),
\]

\[
V_2(\theta) = -2C_2 \cos(2\theta) + 2C_3 \sin(2\theta) - C_4 \cos(\theta) + C_5 \sin(\theta),
\]

\[
V_3(\theta) = -\frac{\sqrt{3}}{3} (3C_2 \sin(2\theta) + 3C_3 \cos(2\theta) - C_1),
\]

\[
V_4(\theta) = 2C_2 \cos(2\theta) - 2C_3 \sin(2\theta) - C_4 \cos(\theta) + C_5 \sin(\theta),
\]

\[
V_5(\theta) = C_2 \sin(2\theta) + C_3 \cos(2\theta) - C_4 \sin(\theta) - C_5 \cos(\theta) + C_1.
\]
For the eigenvectors corresponding to $E_1, \ldots, E_5$, we have respectively

\[
C_1 = \frac{3}{8}, \quad C_2 = 0, \quad C_3 = \frac{1}{8}, \quad C_4 = 0, \quad C_5 = \frac{1}{2},
\]

\[
C_1 = 0, \quad C_2 = \frac{1}{4}, \quad C_3 = 0, \quad C_4 = -\frac{1}{2}, \quad C_5 = 0,
\]

\[
C_1 = \sqrt{6}/8, \quad C_2 = 0, \quad C_3 = -\sqrt{6}/8, \quad C_4 = 0, \quad C_5 = 0,
\]

\[
C_1 = 0, \quad C_2 = \frac{1}{4}, \quad C_3 = 0, \quad C_4 = -\frac{1}{2}, \quad C_5 = 0,
\]

\[
C_1 = \frac{3}{8}, \quad C_2 = 0, \quad C_3 = \frac{1}{8}, \quad C_4 = 0, \quad C_5 = -\frac{1}{2}.
\]

So the eigenvectors are

\[
\begin{bmatrix}
\frac{3}{8} + \frac{1}{8} \cos (2\theta) + \frac{1}{2} \cos (\theta) \\
\frac{1}{4} \sin (2\theta) + \frac{1}{2} \sin (\theta) \\
\frac{\sqrt{6}}{8} (1 - \cos (2\theta)) \\
-\frac{1}{4} \sin (2\theta) + \frac{1}{2} \sin (\theta) \\
\frac{3}{8} + \frac{1}{8} \cos (2\theta) - \frac{1}{2} \sin (\theta)
\end{bmatrix},
\begin{bmatrix}
-\frac{1}{4} \sin (\theta) - \frac{1}{4} \sin (2\theta) \\
\frac{1}{2} \cos (\theta) + \frac{1}{4} \cos (2\theta) \\
\frac{\sqrt{6}}{4} \sin (2\theta) \\
\frac{1}{4} \cos (\theta) - \frac{1}{4} \cos (2\theta) \\
\frac{1}{2} \sin (\theta) - \frac{1}{4} \sin (2\theta)
\end{bmatrix},
\begin{bmatrix}
\frac{\sqrt{6}}{8} (1 - \cos (2\theta)) \\
-\frac{\sqrt{6}}{4} \sin (2\theta) \\
\frac{1}{4} (3 \cos (2\theta) + 1) \\
\frac{\sqrt{6}}{8} \sin (2\theta) \\
\frac{3}{8} + \frac{1}{8} \cos (2\theta) + \frac{1}{2} \cos (\theta)
\end{bmatrix},
\begin{bmatrix}
-\frac{1}{4} \cos (2\theta) + \frac{1}{2} \cos (\theta) - \frac{\sqrt{6}}{4} \sin (2\theta) \\
\frac{1}{4} \cos (2\theta) + \frac{1}{2} \cos (\theta) \\
\frac{1}{4} \sin (2\theta) + \frac{1}{4} \sin (2\theta) \\
-\frac{1}{4} \cos (2\theta) - \frac{1}{2} \sin (\theta) \\
\frac{3}{8} + \frac{1}{8} \cos (2\theta) + \frac{1}{2} \cos (\theta)
\end{bmatrix},
\begin{bmatrix}
\frac{\sqrt{6}}{8} (1 - \cos (2\theta)) \\
-\frac{\sqrt{6}}{4} \sin (2\theta) \\
\frac{1}{4} (3 \cos (2\theta) + 1) \\
\frac{\sqrt{6}}{8} \sin (2\theta) \\
\frac{3}{8} + \frac{1}{8} \cos (2\theta) + \frac{1}{2} \cos (\theta)
\end{bmatrix}.
\]

$n = 5$ Case

The eigenvalues are $E = -5, -3, -1, 1, 3, 5$. The eigenvector calculations go through as before, with the components of the eigenvectors given as linear sums of cos and sin of $\frac{\theta}{2}, \frac{3\theta}{2}$, and $\frac{5\theta}{2}$. For example the eigenvector correspond-
ing to $E = 5$ is
\[
\begin{bmatrix}
\frac{5}{16} \cos \left( \frac{3\theta}{2} \right) + \frac{5}{8} \cos \left( \frac{\theta}{2} \right) + \frac{1}{16} \cos \left( \frac{5\theta}{2} \right) \\
\frac{3\sqrt{6}}{8} \sin \left( \frac{3\theta}{2} \right) + \frac{\sqrt{6}}{8} \sin \left( \frac{\theta}{2} \right) + \frac{\sqrt{6}}{16} \sin \left( \frac{5\theta}{2} \right) \\
-\frac{\sqrt{15}}{16} \cos \left( \frac{3\theta}{2} \right) + \frac{\sqrt{15}}{16} \cos \left( \frac{\theta}{2} \right) - \frac{\sqrt{15}}{16} \cos \left( \frac{5\theta}{2} \right) \\
\frac{\sqrt{16}}{16} \sin \left( \frac{3\theta}{2} \right) + \frac{\sqrt{16}}{16} \sin \left( \frac{\theta}{2} \right) - \frac{\sqrt{16}}{16} \sin \left( \frac{5\theta}{2} \right) \\
-\frac{3\sqrt{5}}{16} \cos \left( \frac{3\theta}{2} \right) + \frac{3\sqrt{5}}{16} \cos \left( \frac{\theta}{2} \right) + \frac{3\sqrt{5}}{16} \cos \left( \frac{5\theta}{2} \right) \\
-\frac{3\sqrt{5}}{16} \sin \left( \frac{3\theta}{2} \right) + \frac{3\sqrt{5}}{16} \sin \left( \frac{\theta}{2} \right) + \frac{3\sqrt{5}}{16} \sin \left( \frac{5\theta}{2} \right)
\end{bmatrix}.
\]

$n = 6$ Case

The calculations go through as before, with the components of the eigenvectors given as linear sums of cos and sin of $0, \theta, 2\theta,$ and $3\theta$. For example the eigenvector corresponding to $E = 6$ is
\[
\begin{bmatrix}
\frac{1}{32} \cos (3\theta) + \frac{3}{16} \cos (2\theta) + \frac{15}{32} \cos (\theta) + \frac{5}{16} \\
\frac{5\sqrt{6}}{32} \sin (\theta) + \frac{\sqrt{6}}{8} \sin (2\theta) + \frac{\sqrt{6}}{16} \sin (3\theta) \\
-\frac{\sqrt{15}}{16} \cos (2\theta) - \frac{\sqrt{15}}{32} \cos (3\theta) + \frac{15}{16} - \frac{\sqrt{15}}{32} \cos (\theta) \\
-\frac{2\sqrt{5}}{32} \sin (3\theta) + \frac{6\sqrt{5}}{32} \sin (\theta) \\
-\frac{\sqrt{15}}{16} \cos (2\theta) + \frac{\sqrt{15}}{32} \cos (3\theta) - \frac{\sqrt{15}}{32} \cos (\theta) \\
\frac{5\sqrt{6}}{32} \sin (\theta) - \frac{\sqrt{6}}{8} \sin (2\theta) + \frac{\sqrt{6}}{16} \sin (3\theta) \\
\frac{5}{16} - \frac{1}{32} \cos (3\theta) + \frac{3}{16} \cos (2\theta) - \frac{15}{32} \cos (\theta)
\end{bmatrix}.
\]

5 Determination of multi-quanta eigenstates using purely algebraic methods.

In what follows we are using superfixes to denote distinct eigenvectors, e.g. $u^i, v^i$ and $V^i$, the last being the $\theta$-dependent eigenvectors of $H(\theta)$. We consider only the cases $n = 1, 2$ to illustrate the technique, other cases follow easily along the same lines.

$n = 1$

$$
e(\theta) = \begin{pmatrix}
-\frac{1}{2} \sin \theta \\
-\frac{1}{2} (1 - \cos \theta)
\end{pmatrix}, \quad f(\theta) = \begin{pmatrix}
-\frac{1}{2} \sin \theta \\
\frac{1}{2} (1 + \cos \theta)
\end{pmatrix}.$$
\[ \tilde{f} = \frac{1}{2} \begin{pmatrix} 1 & -i \\ -i & -1 \end{pmatrix}. \]

\[ u^1 = \begin{pmatrix} 1 \\ i \end{pmatrix}, \quad u^2 = \tilde{f} u^1 = \begin{pmatrix} 1 \\ -i \end{pmatrix}. \]

Solve

\[ v^1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix} = c_1 \begin{pmatrix} 1 \\ i \end{pmatrix} + c_2 \begin{pmatrix} 1 \\ -i \end{pmatrix} \]

for \( c_1 = c_2 = \frac{1}{2} \).

Then

\[ V^1 = \frac{1}{2} \begin{pmatrix} 1 \\ i \end{pmatrix} e^{-\frac{\theta}{2}} + \frac{1}{2} \begin{pmatrix} 1 \\ -i \end{pmatrix} e^{\frac{\theta}{2}} = \begin{pmatrix} \cos \frac{\theta}{2} \\ \sin \frac{\theta}{2} \end{pmatrix}. \]

Finally

\[ V^2 = f(\theta)v^1(\theta) = \begin{pmatrix} -\sin \frac{\theta}{2} \\ \cos \frac{\theta}{2} \end{pmatrix}. \]

These \( V^1 \) and \( V^2 \) are correct and orthonormal with eigenvalues \(-1\) and \(1\) respectively.

\[ n = 2 \]

\[ e(\theta) = \begin{pmatrix}
-\sin \theta & \frac{1}{\sqrt{2}}(1 + \cos \theta) & 0 \\
-\frac{1}{\sqrt{2}}(1 - \cos \theta) & 0 & \frac{1}{\sqrt{2}}(1 + \cos \theta) \\
0 & -\frac{1}{\sqrt{2}}(1 - \cos \theta) & \sin \theta
\end{pmatrix}, \]

\[ f(\theta) = \begin{pmatrix}
-\sin \theta & -\frac{1}{\sqrt{2}}(1 - \cos \theta) & 0 \\
\frac{1}{\sqrt{2}}(1 + \cos \theta) & 0 & -\frac{1}{\sqrt{2}}(1 - \cos \theta) \\
0 & \frac{1}{\sqrt{2}}(1 + \cos \theta) & \sin \theta
\end{pmatrix}. \]

\[ \tilde{f} = \frac{1}{2} \begin{pmatrix} 2 & -i\sqrt{2} & 0 \\
-i\sqrt{2} & 0 & -i\sqrt{2} \\
0 & -i\sqrt{2} & -2 \end{pmatrix}. \]

\[ u^1 = \begin{pmatrix} 1 \\ i\sqrt{2} \\ -1 \end{pmatrix}, \quad u^2 = \tilde{f} u^1 = \begin{pmatrix} 2 \\ 0 \end{pmatrix}, \quad u^3 = \tilde{f} u^2 = \begin{pmatrix} 2 \\ -2i\sqrt{2} \end{pmatrix}. \]
We could choose a different normalization here but it doesn’t help because it gets sorted at the next stage.

Solve
\[
v^1 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = c_1 \begin{pmatrix} 1 \\ i\sqrt{2} \\ -1 \end{pmatrix} + c_2 \begin{pmatrix} 2 \\ 0 \\ 2 \end{pmatrix} + c_3 \begin{pmatrix} 2 \\ -2i\sqrt{2} \\ -2 \end{pmatrix}
\]
for \(c_1 = c_2 = \frac{1}{4}, c_3 = \frac{1}{8}\).

Then
\[
V^1 = \frac{1}{4} \begin{pmatrix} 1 \\ i\sqrt{2} \\ -1 \end{pmatrix} e^{-i\theta} + \frac{1}{4} \begin{pmatrix} 2 \\ 0 \\ 2 \end{pmatrix} + \frac{1}{8} \begin{pmatrix} 2 \\ -2i\sqrt{2} \\ -2 \end{pmatrix} e^{i\theta} = \begin{pmatrix} \frac{1}{2} (1 + \cos \theta) \\ \frac{1}{\sqrt{2}} \sin \theta \\ \frac{1}{2} (1 - \cos \theta) \end{pmatrix}.
\]

\[
V^2 = \frac{1}{\sqrt{2}} f(\theta) v^1(\theta) = \begin{pmatrix} -\frac{1}{\sqrt{2}} \sin \theta \\ \cos \theta \\ \frac{1}{\sqrt{2}} \sin \theta \end{pmatrix},
\]

\[
V^3 = \frac{1}{\sqrt{2}} f(\theta) v^2(\theta) = \begin{pmatrix} \frac{1}{2} (1 - \cos \theta) \\ -\frac{1}{\sqrt{2}} \sin \theta \\ \frac{1}{2} (1 + \cos \theta) \end{pmatrix}.
\]

It is easy to check that these are orthonormal eigenvectors of \(H(\theta)\) with eigenvalues \(-2, 0\) and \(2\) respectively.

6 Conclusion

We developed general procedures to determine exact eigenstates of mixed quantum-classical Davydov dimer for any value of the amide I quantum number \(n\). We also determined a closed expression for the eigenenergies in this system, namely, eq.(9). In future work, these developments will be applied to the calculation of physical quantities such as the dependence on \(n\) of time-dependent probabilities of excitation in each site, the localization threshold, and absorption spectra.
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