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A truncation/recoupling method for eigenvalues and eigenvectors ideal for parallel computation

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Summary. We review a new truncation/recoupling method to obtain eigenvalues and eigenvectors of an F-mode vibrational Hamiltonian. In particular we focus on the block diagonalization aspects of the method which are ideal for massive parallelization, and we demonstrate this using H_2O_2 as an example. We then present vibrational energies for non-rotating HO_2 and HCN, which illustrate several key advantages of this method.

Key words: Vibrational energies – Quantum eigenvalues

1. Introduction

The existence and further development of parallel computers promises to make a major impact in many areas of theoretical/computational chemistry. Indeed, the way in which new algorithms are developed will be strongly influenced by this computer architecture. In this paper we describe a new approach we have very recently developed for treating polyatomic vibrations which is ideally suited for massive parallel computation.

Before we present this approach we need to remind the general reader of the difficulties in doing "exact" calculations of energies and wavefunctions for the vibrations of a polyatomic molecule. First, recall that even for the simplest case of a non-rotating molecule there are $3N-6$ coupled degrees of freedom, where N is the number of atoms. Thus, for triatomic and tetraatomic systems there are three and six degrees of freedom, respectively. If the vibrational wavefunction Ψ_i is expanded in a direct-product of single-mode orthonormal basis functions:

$$\Psi_i = \sum C^i_{n_1 n_2 n_3 \ldots n_F} \phi^{(1)}_{n_1}(q_1) \phi^{(2)}_{n_2}(q_2) \phi^{(3)}_{n_3}(q_3) \ldots \phi^{(F)}_{n_F}(q_F), \tag{1}$$

where $F = 3N-6$, then the eigenvalue problem:

$$(\mathbf{H}-\mathbf{E})\mathbf{C} = \mathbf{0} \tag{2}$$

can be enormous. To see that, recall that if the upper limits on the F-fold summation in Eq. (1) are $n_1^m, n_2^m, \ldots, n_F^m$, then, if there are no restrictions on the summations, the order of the $\mathbf{H}$ matrix, N_0, is $n_1^m \times n_2^m \times \cdots \times n_F^m$. A very modest value of each upper limit is 10, and thus N_0 equals 10^F, i.e., exponential growth with F. This growth rate is clearly unacceptable for $F > 3$, that is, for tetraatomic and larger molecules. Even for triatomics, the number 10 may be too small for many interesting cases, e.g., isomerizations, highly excited large amplitude motions, bases for reactive scattering, etc. A value of 20 for the upper limit of each summation would imply an **H** matrix of order 8000. There are methods to deal with such large matrices for selected eigenvalues and eigenvectors, and we refer the reader to several recent reviews of them [1, 2]. Even these methods will eventually have difficulties for general $F > 3$ problems.

Clearly, the problem is with the direct-product basis. There are general strategies which have recently been suggested to restrict the size of the number of terms in the basis [3, 4]; however, we don't wish to review them here. We do note that a very promising alternative is to use a direct-product of a mixture of multimode and single-mode basis functions [5]. That is a very promising approach and it is related in spirit to one we have recently considered [6] and which is the subject of this paper.

The method we describe is a non-direct-product representation of the wavefunction that lends itself to an efficient truncation/recoupling scheme. In particular it is ideally suited for massive parallelization. Before we present the method, and illustrations, we note that our approach is similar in spirit to the recent work of Light and co-workers who apply a Discrete Variable Representation (DVR) to triatomic vibrations [7, 8]. That method is also ideally suited for massive parallelization.

To summarize the rest of the paper: the theory of the truncation/recoupling method is presented in the next section, several illustrations of the method are given in Sect. 3, and a summary constitutes Sect. 4.

2. Truncation/recoupling theory

The **H**-matrix in the Heisenberg eigenvalue equation, Eq. (2), can be written as follows:

$$\mathbf{H} = \begin{bmatrix} \mathbf{H}_{1,1} & \mathbf{H}_{1,2} & \cdots & \mathbf{H}_{1,d} & \cdots \\ \mathbf{H}_{2,1} & \mathbf{H}_{2,2} & \cdots & \mathbf{H}_{2,d} & \cdots \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \mathbf{H}_{d,1} & \mathbf{H}_{\mathrm{d},2} & \cdots & \mathbf{H}_{d,d} & \cdots \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \end{bmatrix},$$

that is a matrix of matrices. For the sake of concreteness we associate the submatrices $\mathbf{H}_{dd}$ with two modes which we take to be modes q_1 and q_2 in Eq. (1). The row vector $\boldsymbol{d}$ is an ordered set of integers referring to the remaining $F-2$ modes, i.e.,

$$\boldsymbol{d} = (n_3\, n_4\, n_5 \cdots n_F).$$

As usual, an element of **H** is given by

$$H_{n'_1 n'_2 \boldsymbol{d}, n_1 n_2 \boldsymbol{d}} = \left\langle \prod_{i'=3}^{F} \phi^{(i')}_{n'_i} \middle| \langle \phi^{(1)}_{n_{1'}} \phi^{(2)}_{n_{2'}} | H | \phi^{(1)}_{n_1} \phi^{(2)}_{n_2} \rangle \middle| \prod_{i=3}^{F} \phi^{(i)}_{n_i} \right\rangle,$$

where H is the exact Hamiltonian operator.

Next we re-write **H** as:

$$\mathbf{H} = \mathbf{H}_0 + \mathbf{H}_1,$$

where

$$\mathbf{H}_0 = \begin{bmatrix} \mathbf{H}_{1,1} & \mathbf{0} & \cdots & \mathbf{0} & \cdots \\ \mathbf{0} & \mathbf{H}_{d,1} & \cdots & \mathbf{0} & \cdots \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \mathbf{0} & \mathbf{0} & \cdots & \mathbf{H}_{d,d} & \cdots \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \end{bmatrix},$$

and

$$\mathbf{H}_1 = \begin{bmatrix} \mathbf{0} & \mathbf{H}_{1,2} & \cdots & \mathbf{H}_{d,d} & \cdots \\ \mathbf{H}_{2,1} & \mathbf{0} & \cdots & \mathbf{H}_{2,d} & \cdots \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \mathbf{H}_{d,1} & \mathbf{H}_{d,2} & \cdots & \mathbf{0} & \cdots \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \end{bmatrix}.$$

A key step in the truncation/recoupling method is the diagonalization of $\mathbf{H}_0$, which even though it may be an enormous matrix, can be accomplished fairly readily due to its block diagonal structure. Indeed, the task of diagonalizing $\mathbf{H}_0$ is ideally suited for massive parallelization. To make this clear, we digress from the truncation/recoupling method and focus on a simple example.

H_2O_2

An interesting system which lends itself to the above decomposition of **H** is hydrogen peroxide. We associate the coordinates q_1 and q_2 with the symmetric and antisymmetric OH normal modes, and q_3–q_6 with the remaining normal modes. The harmonic frequencies of these modes from a recent *ab initio* calculation [9] are given in Table 1. As seen, we have chosen the two high frequency OH stretches to be represented by the submatrices $\mathbf{H}_{d,d}$. We now wish to determine the order of $\mathbf{H}_0$, N_0, and the number of blocks, N_b, in $\mathbf{H}_0$, for several cases of interest. Suppose we decide to include all states $\boldsymbol{d} = n_3 n_4 n_5 n_6$ such that the uncoupled harmonic excitation energies $n_3\omega_3 + n_4\omega_4 + n_5\omega_5 + n_6\omega_6$ are below a threshold value E_{th}. (The number of states is equal to the number of blocks N_b.) Also, we assume that the order of $\mathbf{H}_{d,d}$ is 400, which is a reasonable size to obtain high energy eigenvalues of a two-mode Hamiltonian matrix. We have tabulated the number of blocks and the order of $\mathbf{H}_0$ (and **H**) for four values of E_{th} in Table 2. The order is clearly out of the range by orders of magnitude for any computer. However, the number of blocks in $\mathbf{H}_0$ is well within the maximum number of processors of existing parallel computers, e.g., the CM-2 connection machine, which has a maximum of 65536 processors [10]. Thus, diagonalization of $\mathbf{H}_0$ which is equivalent to diagonalizing N_{b} 400×400 matrices can be done on existing parallel computers.

We now continue with our brief description of the truncation/recoupling

Table 1. Harmonic normal mode frequencies (in cm^{-1}) of H_2O_2[a] (using non-conventional notation)

ω_1 (antisym OH str)	3820
ω_2 (sym OH str)	3816
ω_3 (sym HOO bnd	1429
ω_4 (antisym HOO bnd)	1328
ω_5 (OO str)	887
ω_6 (trosion)	383

[a] From Ref. [9]

Table 2. The number of blocks N_b in $\mathbf{H}_0$, and the order of $\mathbf{H}_0$ (and $\mathbf{H}$), N_0, for H_2O_2 for four values of the threshold energy (in cm^{-1}) E_{th}

E_{th}	N_b	N_0
15,000	1810	7.24×10^5
20,000	6716	2.69×10^6
25,000	17964	7.19×10^6
30,000	39530	1.58×10^7

theory. The new two-mode "dressed" basis is obtained from diagonalization of $\mathbf{H}_0$, and is denoted $\chi_j^d(q_1, q_2)$. These dressed eigenfunctions are combined with the zero-order, single-mode ones to yield a new, non direct-product basis:

$$\Psi_j^d(q_1, q_2, \ldots, q_F) = \phi_{n_3}^{(3)}(q_3) \cdots \phi_{n_F}^{(F)}(q_F)\chi_j^d(q_1, q_2),$$

in terms of which the exact wavefunctions Ψ_i are expanded, i.e.:

$$\Psi_i(q_1, q_2, \ldots, q_F) = \sum_{d_j} a_{dj}^i \Psi_i^d(q_1, q_2, \ldots, q_F).$$

The terminology "dressed" to describe the two-mode basis seems appropriate since the two-mode Hamiltonian $\mathbf{H}$ is "dressed" by a given zero-order state $\phi_{n_3}^{(3)}(q_3) \cdots \phi_{n_F}^{(F)}(q_F)$. A very important property of the Ψ_i^d (which can be seen by inspection) is that they form an orthonormal set of functions, i.e.:

$$\langle \Psi_{j'}^d | \Psi_j^d \rangle = \delta_{dd}\delta_{j'j}.$$

The full Hamiltonian in the new F-mode basis has the following structure

$$\mathbf{H}^t = \begin{bmatrix} \mathbf{E}_0^1 & \mathbf{H}_{1,2}^t & \cdots & \mathbf{H}_{d,d}^t & \cdots \\ \mathbf{H}_{2,1}^t & \mathbf{E}_0^2 & \cdots & \mathbf{H}_{2,d}^t & \cdots \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \mathbf{H}_{d,1}^t & \mathbf{H}_{d,2}^t & \cdots & \mathbf{E}_0^d & \cdots \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \end{bmatrix},$$

where the diagonal blocks $\mathbf{E}_0^1, \mathbf{E}_0^2, \ldots \mathbf{E}_0^d$, are diagonal matrices of the eigenvalues of $\mathbf{H}_0$. In principle these blocks are the same order as the blocks in $\mathbf{H}_0$. However, a major reduction in their order, and hence the overall order of $\mathbf{H}^t$ can be made if basis functions Ψ_j^d with energies below a cutoff energy are used in the final re-coupling. For this truncation of the basis to be effective, it is necessary that the zero-order energies E_0 be close to the exact ones. An investigation of this is made below for two examples, HO_2 and HCN.

3. Triatomic examples

We consider two triatomic examples to illustrate some of the results we have obtained with the dressed state truncation/recoupling method. We use mass-scaled Jacobi coordinates, $\boldsymbol{R}_1$ and $\boldsymbol{R}_2$, which are the mass-scaled position vectors of the atom with respect to the center of mass of the diatom, and the mass scalled diatom internuclear position vector. The quantity γ is defined to be the angle between those vectors.

In the applications below R_1, γ, and R_2 play the roles of q_1, q_2, and q_3, respectively. The basis functions for these modes are eigenfunctions of reference Hamiltonians which are given by:

$$h^{(1)} = -\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial R_1^2} + V(R_1 R_2^0, \gamma^0),$$

$$h^{(2)} = B_0 j_0^2 + V(R_1^0, R_2^0, \gamma),$$

$$h^{(3)} = -\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial R_2^2} + V(R_1^0, R_2, \gamma).$$

where R_1^0, R_2^0, and γ^0 are constants.

The modes R_1 and γ are coupled, and the dressed Schrödinger equation for the eigenfunctions $\chi_j^{n_3}(R_1, \cos\gamma)$ is:

$$(H^{n_3} - E_{j0}^{n_3})\chi_j^{n_3}(R_1, \gamma) = 0,$$

where

$$H^{n_3} = -\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial R_1^2} + \langle\phi_{n_3}^{(3)}|B(R_1, R_2)|\phi_{n_3}^{(3)}\rangle j_0^2 + \langle\phi_{n_3}^{(3)}|V(R_1, R_2, \gamma)|\phi_{n_3}^{(3)}\rangle,$$

where $B(R_1, R_2)$ is the inverse moment of inertia, j_0^2 is the diatom angular momentum operator squared in a body-fixed frame, $V(R_1, R_2, \gamma)$ is the full potential, and $\phi_{n_3}^{(3)}$ is an eigenfunction of $h^{(3)}$. The eigenfunctions $\chi_j^{n_3}(R_1, \cos\gamma)$ are expanded in a direct-product of the eigenfunctions of $h^{(1)}$ and $h^{(2)}$.

We now consider two examples, HO_2 and HCN.

HO_2

As a first example, consider non-rotating HO_2 in mass-scaled Jacobi coordinates. R_1 is the mass-scaled distance of H with respect to the center of mass of O_2 and R_2 is the mass-scaled O_2 internuclear distance. The potential we used is the double-many-body-expansion of Verandas and Brandão [11] fit to the *ab inito* calculations of Melius and Blint [12]. An equipotential contour diagram of the surface in physical coordinates (with R_2 fixed) is shown in Fig. 1. Clearly, there is substantial R_1–γ correlation. Interestingly though, we examined a contour plot in R_1–R_2 for fixed γ and found very little correlation, except at energies above dissociation. This incicates that the choice of modes to couple, R_1 and γ, is the correct one.

We calculated zero-order, dressed eigenvalues using a fairly large direct-product basis for the R_1 and γ modes. The basis in these two modes was a direct product of stretching and bending functions which are eigenfunctions of $h^{(1)}$ and $h^{(2)}$. The reference configuration (R_1^0, R_2^0, γ^0) is the HO_2 equilibrium position (which is bent, $\gamma^0 = 45$ deg). The dressed, zero-order eigenvalues were obtained by diagonalizing sixteen Hamiltonians, H^{n_3}, using a direct-product basis of order 440, which consisted of 20 stretching functions, and 22 bending functions.

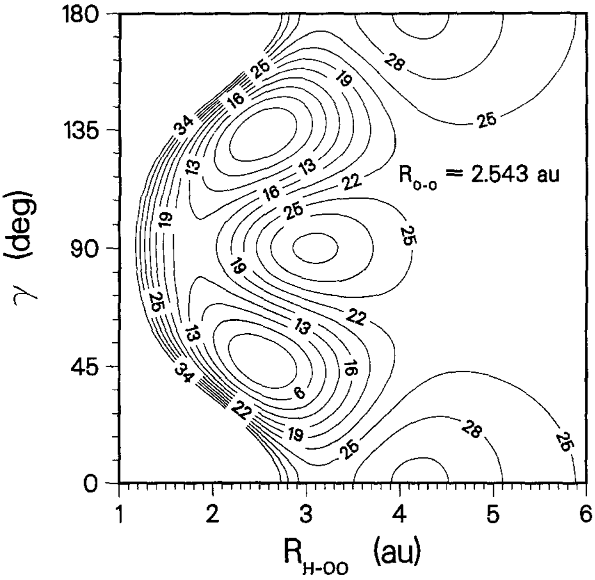

Fig. 1. Equipotential contour plot of the HO_2 potential (from Ref. [11]) in physical coordinates, i.e., the distance of H to the center of mass of O_2 and the angle γ (see text) for a fixed O–O bond length. The contour values are in units of 1000 cm^{-1}

The truncation/recoupling calculations included all zero-order states with energies below 30,000 cm^{-1}. This resulted in a final Hamiltonian matrix of order 932, and, based on convergence studies with smaller bases, the eigenvalues are accurate to within several cm^{-1} or less for energies up to roughly 14,000 cm^{-1}. These calculations are for even parity states. Odd parity states were also calculated, separately. The splittings between the even and odd parity states and further details of the calculations will be given elsewhere [13].

The results of some of these calculations for states below the isomerization barrier (which is 12092 cm^{-1} above the HO_2 minimum) are given in Table 3. The vibrational states are denoted using conventional normal-mode notation (n_{OO}, n_b, n_{OH}), where the quantum numbers refer to the OO stretch, the bend, and the OH stretch. As seen, the zero-order energies are quite close to the converged truncation/recoupling energies. Note, that the zero-order energies are not upper bounds to the exact ones, and so the negative differences should not be surprising. An important aspect of this comparison is that the accuracy of the dressed zero-order energies remains constant as the energy increases. These results are quite similar to previous ones we have reported for HCO, but in that case for all the bound states [6].

HCN

We calculated truncation/recoupling energies for non-rotating HCN up to 15252 cm^{-1}, using the potential surface of Murrell et al. [14].

In this example, R_1 is the mass-scaled distance of H to the center of mass of CN and R_2 is the mass-scaled CN internuclear distance. The two modes coupled are R_1 and γ, as in HO_2. As seen from an equipotential contour diagram in physical coordinates (with R_{CN} fixed at its equilibrium value) shown in Fig. 2,

Table 3. Truncation/recoupling, $E_{t/r}$, and zero-order dressed state, E_0, and their difference (in cm^{-1}) for non-rotating HO_2

State ($n_{OO}n_bn_{OH}$)	E_0	$E_{t/r}$	$E_0 - E_{t/r}$
(0, 0, 0)	3051.2	3049.5	1.7
(1, 0, 0)	4285.4	4277.3	8.1
(0, 1, 0)	4878.2	4879.7	−1.5
(2, 0, 0)	5501.4	5486.8	14.6
(0, 0, 1)	5989.6	5980.6	9.0
(1, 1, 0)	6100.0	6092.7	7.3
(0, 2, 0)	6651.9	6654.4	−2.5
(3, 0, 0)	6699.1	6678.4	20.7
(2, 1, 0)	7226.0	7206.8	19.2
(1, 0, 1)	7302.9	7287.1	15.8
(0, 1, 1)	7765.4	7764.3	1.1
(1, 2, 0)	7860.6	7850.7	9.9
(4, 0, 0)	7879.6	7853.5	26.1
(0, 3, 0)	8369.3	8372.8	−3.5
(2, 0, 1)	8444.8	8412.7	32.1
(3, 1, 0)	8486.9	8464.2	22.7
(0, 0, 2)	8850.1	8827.4	22.7
(1, 1, 1)	8986.9	8971.1	15.8
(5, 0, 0)	9047.8	9015.3	32.5
(2, 2, 0)	9050.5	9030.7	19.8
(0, 2, 1)	9477.8	9480.3	−2.5
(1, 3, 0)	9566.0	9552.6	13.4
(3, 0, 1)	9645.8	9594.3	51.5
(4, 1, 0)	9653.4	9630.5	22.9
(0, 4, 0)	10029.6	10034.0	−4.4
(1, 0, 2)	10088.9	10048.7	40.2

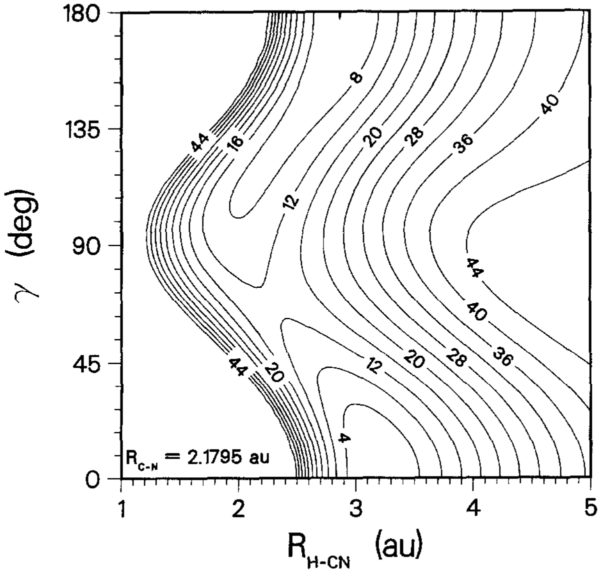

Fig. 2. Same as Fig. 1 but for HCN (from Ref. [14]), where $R_{\text{H-CN}}$ is the distance of H to the center of mass of CN

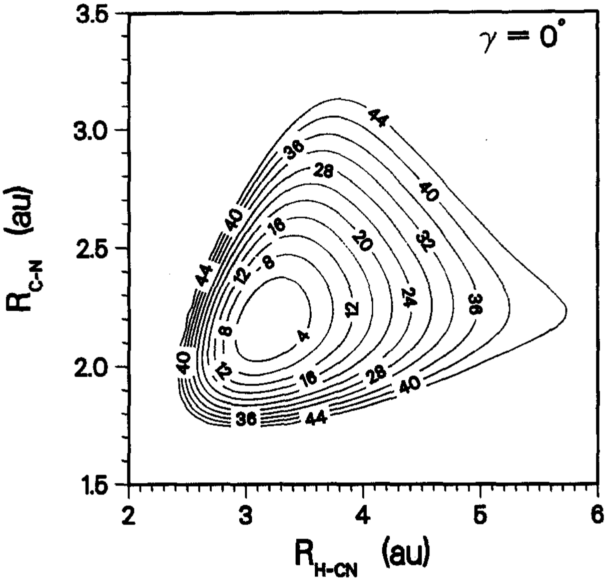

Fig. 3. Equipotential contour plot for HCN in terms of physical radial coordinates for the linear configuration. Contour values are in units of 1000 cm^{-1}

HCN has even more R_1–γ correlation than HO_2. The two minima, corresponding to linear HCN and linear HNC have quite different values of $R_{H\text{-}CN}$. Also, there is considerable R_1–R_2 correlation, as seen in Fig. 3. [In a separate study, we found that the R_1–R_2 correlation can be very effectively accounted for by a simple rotation of the (R_1, R_2) coordinates to new coordinates (Q_1, Q_2) [15].] Thus, we do not expect the zero-order dressed energies to be as accurate for HCN (using R_1 and R_2) as they were for HO_2 (and HCO). And, indeed, as seen in Table 4, that is the case. The differences are roughly a factor of 10 larger than in HO_2. Even so, the truncation/recoupling results in this table, which used nine CN basis functions, are in excellent agreement with previous calculations of Bačić and Light [16], (with a few exceptions for states involving CN excitation), and in very good agreement with previous calculations of Brunet et al. [17]. We note that the order of the final truncated *H*-matrix was 689, whereas the direct-product basis used to obtain the dressed eigenfunctions would have resulted in an *H*-matrix of order 13,068.

Finally, we note that truncation/recoupling calculations can be done with rotated R_1 and R_2 coordinates, and we anticipate that much more accurate zero-order energies would result.

4. Conclusion

A truncation/recoupling method to obtain eigenvalues and eigenvectors of large matrices has been reviewed. In this method a major step involves diagonalization of a very large, block diagonal, matrix. The blocks are of modest size, and thus this diagonalization is ideally suited for massive parallel computation. We described an example calculation of the vibrational energies of H_2O_2, where it was clearly shown that the conventional direct-product method would be prohibitive for existing, and future computers. However, the calculation should be quite feasible for machines such as the *Connection Machine*.

Table 4. Low energy dressed state and truncation/recoupled ($E_{t/r}$) eigenvalues (in cm^{-1}) for non-rotating HCN

State (HCN) or [HNC]	$E_{t/r}$	E_0	$E_0 - E_{t/r}$
(0, 0, 0)	3483.3	3524.7	41.4
(0, 2, 0)	4901.5	4935.5	34.0
(1, 0, 0)	5580.3	5813.4	233.1
(0, 4, 0)	6289.7	6319.6	30.0
(0, 0, 1)	6801.8	6716.1	−85.7
(1, 2, 0)	6991.9	7201.3	209.4
[0, 0, 0]	7291.2	7347.0	55.8
(0, 6, 0)	7644.3	7672.8	28.5
(2, 0, 0)	7657.1	8079.8	422.7
(0, 2, 1)	8190.2	8108.3	−81.9
[0, 2, 0]	8234.2	8293.1	58.9
(1, 4, 0)	8374.0	8565.4	191.5
(1, 0, 1)	8884.9	8990.0	105.0
(0, 8, 0)	8960.8	8997.5	36.8
(2, 2, 0)	9061.8	9166.1	104.4
[0, 4, 0]	9108.5	9444.8	336.3
[1, 0, 0]	9321.3	9471.9	150.6
(0, 4, 1)	9548.4	9545.5	−2.8
(3, 0, 0)	9715.9	9798.9	83.1
(1, 6, 0)	9722.9	9864.1	141.2
[0, 6, 0]	9810.6	9901.1	90.5
(0, 0, 2)	10014.9	10264.9	250.1
[0, 8, 0]	10132.5	10265.0	132.5
(0, 10, 0)	10233.6	10324.4	90.9
[1, 2, 0]	10254.5	10366.8	112.4
(1, 2, 1)	10267.0	10470.0	203.0
(2, 4, 0)	10436.6	10704.5	268.0
[0, 10, 0]	10530.8	10788.7	257.9
(0, 6, 1)	10872.9	10802.9	−70.0
[0, 0, 1]	10923.8	10891.4	−32.4
(2, 0, 1)	10951.2	11172.2	221.0
[0, 12,0]	11021.6	11203.4	181.8
(1, 8, 0)	11034.3	11230.9	196.6
(3, 2, 0)	11113.0	11256.8	143.8
[1, 4, 0]	11123.6	11328.1	204.5
[2, 0, 0]	11333.0	11489.7	156.8
(0, 2, 2)	11373.0	11666.4	293.4
(0, 12, 0)	11454.7	11710.1	255.4
[0, 14, 0]	11576.9	11720.2	143.3
(1, 4, 1)	11618.5	11813.0	194.5
(4, 0, 0)	11760.6	11813.7	53.1
(2, 6, 0)	11779.7	12027.1	247.5
[0, 2, 1]	11834.0	12073.8	239.8
[1, 6, 0]	11842.3	12096.3	253.9
(1, 0, 2)	12084.5	12106.9	22.4

Actual calculations of vibrational energies using the truncation/recoupling method were presented for HO_2 and HCN. Although the method worked well for HCN we noted that the zero-order energies were less accurate than the corresponding ones for HO_2. This was due to substantially more radial-radial (R_1–R_2) correlation in HCN than in HO_2.

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