Variational collocation for systems of coupled anharmonic oscillators

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Abstract

By means of a collocation approach based on little sinc functions (LSF), we obtain accurate eigenvalues and eigenfunctions of the stationary Schrödinger equation for systems of coupled oscillators. Adjustable parameters introduced by means of scaling and rotation of the coordinates improve the rate of convergence of the approach. A careful comparison with the results published earlier by other authors shows the advantages of the present approach.

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(Some figures in this article are in colour only in the electronic version.)

1. Introduction

Coupled anharmonic oscillators have proved useful for modelling a wide variety of physical problems, such as, for example, the vibrations of polyatomic molecules \cite{1–3}. For this reason, there has been great interest in the calculation of their eigenvalues and eigenfunctions \cite{4–22} (and references therein).

In order to obtain accurate eigenvalues and eigenfunctions of the Schrödinger equation for coupled anharmonic oscillators, we propose a collocation approach that allows the discretization of a $D$-dimensional region by means of a particular set of functions called little sinc functions (LSF) \cite{25–29}. LSF were proposed by Baye \cite{30} who called them ‘first sinc basis’. This basis set proved useful for the accurate variational treatment of the one-dimensional Schrödinger equation \cite{25}, the representation of non-local operators on a uniform grid for the solution of the relativistic Salpeter equation \cite{26}, and for the accurate treatment of the Helmholtz equation on arbitrary two-dimensional domains, both for the homogeneous \cite{27} and inhomogeneous \cite{28} cases. Recently, we investigated the practical utility of four sets of LSF \cite{29} with different boundary conditions that include the original set \cite{25} as a particular case. Here, we restrict ourselves to the LSF set with Dirichlet boundary conditions \cite{25}.

In this paper, we propose an alternative variational method for the calculation of eigenvalues and eigenfunctions of coupled anharmonic oscillators. We develop the approach in section 2; in section 3, we consider four coupled harmonic oscillators that are useful for testing our approach because the model is exactly solvable. In sections 4–6, we obtain the eigenvalues of two, three and four coupled anharmonic oscillators, respectively. In each case, we compare our results with those obtained earlier by other authors using different approaches. Finally, in section 7, we draw conclusions.

2. The method

To make our discussion self-contained, we outline the main features of our approach, starting with the set of functions that are used for discretization. An LSF is an approximate representation of the Dirac delta function in terms of the wave functions of a particle in a box of size $2L$:

\[ s_k(h, N, x) = \frac{1}{2N} \left\{ \frac{\sin((2N+1)\chi_-(x))}{\sin\chi_-(x)} - \frac{\cos((2N+1)\chi_+(x))}{\cos\chi_+(x)} \right\}, \]

where $\chi_\pm(x) = \frac{\pi}{2Nh}(x \pm kh)$. The index $k$ takes all the integer values between $-N/2+1$ and $N/2-1$, where $N$ is an
even integer. The LSF $s_k$ is peaked at $x_k = 2Lk/N = kh$, $h$ being the grid spacing and $2L$ the total extension of the interval where the function is defined. These LSF satisfy $s_k(h, N, x_j) = \delta_{kj}$ and are orthogonal

$$\int_{-L}^{L} s_k(h, N, x)s_j(h, N, x)dx = h\delta_{kj}.$$  

It follows from those properties of the LSF that we can approximate a function defined on $x \in (-L, L)$ as

$$f(x) \approx \sum_{k=-N/2+1}^{N/2-1} f(x_k) s_k(h, N, x).$$  

(2)

In a similar way, we can also represent a derivative of an LSF as

$$\frac{ds_k(h, N, x)}{dx} \approx \sum_{j} \frac{ds_k(h, N, x)}{dx} \bigg|_{x=x_j} s_j(h, N, x)$$

$$= \sum_{j} c^{(1)}_{kj} s_j(h, N, x),$$

(3)

$$\frac{d^2 s_k(h, N, x)}{dx^2} \approx \sum_{j} \frac{d^2 s_k(h, N, x)}{dx^2} \bigg|_{x=x_j} s_j(h, N, x)$$

$$= \sum_{j} c^{(2)}_{kj} s_j(h, N, x),$$

(4)

where the analytical expressions for the coefficients $c^{(r)}_{kj}$ have been given elsewhere [25].

Although equation (2) is not exact, we can make the error of that representation of the function $f(x)$ as small as possible by simply increasing the value of $N$, as discussed in our earlier paper [25]. The effect of this approximation is the discretization of the continuous interval $2L$ into a set of $N - 1$ uniformly spaced points, $x_j$. For example, the application of this approach to a one-dimensional eigenvalue problem results in the diagonalization of an $(N - 1) \times (N - 1)$ matrix.

An appropriate basis set for a $D$-dimensional problem is given by the direct product of one-dimensional LSF that generates a uniform grid with spacing $h$ (in some particular cases, it may be more convenient to consider different spacings in different directions). A set of $D$ integers $(k_1, k_2, \ldots, k_D)$ completely specifies the location of a given point inside the hyper-volume. However, with the purpose of constructing Hamiltonian matrices, it is convenient to identify one such point with just a single integer $K_D$ that takes all the values between 1 and $(N - 1)^D$.

In this paper, we only consider Hamiltonian operators of the form

$$\hat{H} = T(\hat{p}_1, \hat{p}_2, \ldots, \hat{p}_D) + V(\hat{x}_1, \hat{x}_2, \ldots, \hat{x}_D),$$

(5)

where $T$ is a polynomial of second degree and $V$ is a polynomial function of the coordinates that is bounded from below. We assume that the eigenfunctions $\psi_n(x_1, \ldots, x_D)$ are defined in a $D$-dimensional hypercube $\Omega$ of side $L$ and satisfy Dirichlet boundary conditions on the frontier $\partial\Omega$.

By means of the discretization based on the direct product of LSF outlined above, we obtain a Hamiltonian matrix of the form

$$H_{k_1,k_2,\ldots,k_D} = T_k k_1 \delta_{k_1,k_1} \delta_{k_2,k_2} \cdots \delta_{k_D,k_D} + \cdots + \delta_{k_1,k_1} \delta_{k_2,k_2} \cdots \delta_{k_D,k_D} T_k + \sum_{k_1,k_2,\ldots,k_D} T_k k_1 k_2 \cdots k_D,$$  

(6)

where $k_i$ and $k'_i$ range from $-N/2 + 1$ to $N/2 - 1$. In order to apply well-known matrix operations, we express the $2D$ labels $k_i$ and $k'_i$ in terms of just two $\tilde{K}_D$ and $\tilde{K}'_D$ and obtain an $(N - 1)^D \times (N - 1)^D$ matrix representation of the Hamiltonian operator. We expect that its eigenvalues and eigenvectors tend to the energies and wave functions, respectively, of the Hamiltonian operator as $N$ increases. Note that the potential part of this matrix is diagonal, whereas the kinetic one is sparse. These two features facilitate the numerical treatment of multidimensional problems as we will see in what follows.

In principle, we have two adjustable parameters: $N$ and $L$, but we can bind them together by means of the variational method. As discussed elsewhere [25], it is convenient to set the optimal value of the scale parameter $L$ in such a way that the trace of the Hamiltonian matrix is minimum. As shown earlier [25], we may obtain general expressions for the trace of the kinetic and potential parts of the Hamiltonian matrix. In the former case, we obtain

$$\mathcal{K}_{n}^{(D)} = D(N - 1)^{D - 1} - \frac{h^2}{2m} \sum_{k=-N/2+1}^{N/2-1} c_{k}^{(2)}$$

$$= D(N - 1)^{D - 1} \mathcal{K}_{n}^{(1)},$$

(7)

where $\mathcal{K}_{n}^{(1)}$ is the one-dimensional trace already calculated earlier [25]. The trace of the potential part is given by

$$\mathcal{V}_{n}^{(D)} = \sum_{k_1, \ldots, k_D} V(x_1, \ldots, x_D)$$

$$\approx \frac{1}{h^D} \int_{-L}^{L} dx_1 \cdots \int_{-L}^{L} dx_D V(x_1, \ldots, x_D),$$

(8)

where $h = 2L/N$. We may use the integral when $N \gg 1$ and the sum for moderate values of $N$.

The trace of the Hamiltonian matrix is therefore an analytic function of both $N$ and $L$. The optimal value of the latter $L_{\text{PMS}}(N)$ is obtained from the minimum of the trace with respect to $L$. Here, PMS stands for principle of minimal sensitivity [31] and the resulting Hamiltonian matrix depends only on $N$. Note that for potentials that are polynomial functions of the coordinates, such as those considered in this paper, the different scaling behaviour of $\mathcal{K}_{n}^{(D)}$ and $\mathcal{V}_{n}^{(D)}$ with respect to $L$ ensures the existence of a minimum in the trace. As an example, we generalize the result of equation (50) of [25] to the case of a $D$-dimensional harmonic oscillator $V(x_1, \ldots, x_D) = \frac{1}{2}(x_1^2 + \cdots + x_D^2)$. In this case, setting $h = m = 1$, we find that

$$h_{\text{PMS}} = \frac{2L_{\text{PMS}}}{N} \approx \left( \frac{2^{3D-1}}{3^{D-1}} \right)^{1/(2(D+1))} \left( \frac{\pi}{N^D} \right)^{1/(D+1)},$$

(9)

which reduces to the result derived earlier for $D = 1$ [25].
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Other authors have already resorted earlier to the minimization of the trace of the Hamiltonian matrix as a way of obtaining optimal values of the variational parameters in quantum-mechanical calculations [32, 33].

The construction of the kinetic-energy matrix \( T \) is the time-consuming part of the process of building the Hamiltonian matrix \( H \). However, in the problems discussed here, the form of \( T \) depends only on \( N \) and \( D \) and is suitable for several models with different potential-energy functions \( V \). We can thus take advantage of the fact that the calculation of the matrix \( V \) is faster because it is diagonal with only \((N-1)^D \) elements.

3. Coupled harmonic oscillators

In order to test the accuracy and rate of convergence of our approach, we first consider a set of \( D \) coupled harmonic oscillators given by the Hamiltonian operator

\[
H = \sum_i \left( -\frac{1}{2} \frac{\partial^2}{\partial x_i^2} + \frac{1}{2} x_i^2 \right) + \frac{1}{2} \sum_{ij} v_{ij} x_i x_j, \quad (10)
\]

where \( v_{ij} = v_{ji} \). One can easily solve the Schrödinger equation and obtain the eigenvalues exactly:

\[
E_n = \sum_i \sqrt{1 + \lambda_i} \left( n_i + \frac{1}{2} \right), \quad (11)
\]

where \( n_i = 0, 1, \ldots, i = 1, 2, \ldots, D \) are the harmonic oscillator quantum numbers and \( \lambda_i \) are the eigenvalues of the symmetrical matrix with elements \( v_{ij} \).

The value of \( L \) that makes the trace of the Hamiltonian matrix a minimum is given by

\[
L_{\text{PMS}} = \sqrt{\frac{\pi N}{2}} \left[ 1 + \frac{3}{8N} + \frac{53}{128N^2} + O \left( \frac{1}{N^3} \right) \right], \quad (12)
\]

and is shown by the solid curve in figure 1. The dashed curve, on the other hand, shows the approximate value of \( L_{\text{PMS}} \) given by the substitution of the integral for the sum of the potential part as indicated above:

\[
L_{\text{PMS}} = \sqrt{\frac{\pi N}{2}} \left[ 1 - \frac{9}{8N} - \frac{3}{128N^2} + O \left( \frac{1}{N^3} \right) \right]. \quad (13)
\]

Note that the leading term is correctly reproduced by this approximate formula as expected from the fact that the sum becomes the integral when \( N \to \infty \). The plus signs in the figure are the actual minima of the trace used to obtain the results of table 1.

Table 1 shows the energies of the ground and first excited states of \( D = 4 \) harmonic oscillators with \( v_{ij} = (1 - \delta_{ij})/3 \) for increasing matrix dimension (increasing \( N \)). We appreciate that the rate of convergence of the present method is satisfactory for the treatment of coupled oscillators.

It may be useful to observe that the kinetic and potential contributions to the trace of the Hamiltonian have different dependence on \( L \): the first term goes like \( L^{-2} \), whereas the second term, for the polynomial potential that we are considering here, goes like \( L^{2} \). This ensures the presence of a minimum, whose location depends on \( N \), as one can see using the expressions given in equations (7) and (8).

![Figure 1. \( L_{\text{PMS}} \) as a function of \( N \) for four coupled harmonic oscillators like (10) with eigenvalues in table 1.](image)

| \( N \) | \( E_0 \) | \( E_1 \) | \( E_2 \) |
|------|------|------|------|
| 6    | 1.929 802495 | 2.755 212192 | 3.346 193354 |
| 8    | 1.931 801216 | 2.748 861410 | 3.346 218192 |
| 10   | 1.931 851103 | 2.748 382295 | 3.346 079656 |
| 12   | 1.931 851707 | 2.748 350435 | 3.346 066304 |
| 14   | 1.931 851659 | 2.748 348376 | 3.346 065292 |
| 16   | 1.931 851653 | 2.748 348243 | 3.346 065220 |

Exact 1.931 851653 2.748 348234 3.346 065215
and, consequently, its construction does not require much time.

Once the matrix has been generated one should calculate the eigenvalues and eigenvectors of interest. For matrices of modest size, we simply use standard diagonalization routines. On the other hand, for large matrices it is more practical to resort to iterative algorithms that extract a selected eigenvalue/eigenvector because they commonly require less computer memory. Such methods require an initial vector guess, and after some iterations produce the eigenvector corresponding to the lowest eigenvalue with prescribed tolerance. We have found a conjugate gradient (CG) algorithm sufficiently efficient for the present calculations. A simple modification of this algorithm is suitable for the calculation of arbitrary eigenvalues/eigenvectors [34–36]. In fact, we can easily obtain the eigenvalue of the matrix M closest to λ by application of the CG algorithm to the modified matrix \( \tilde{M} \equiv (M - λI)^2 \). The algorithm works as in the case of the lowest eigenvalue except that the convergence rate is typically smaller.

Another important issue is the guess of the initial vector. In the case of a collocation method, the vector elements are the values of a function at the chosen grid points. If the Hamiltonian operator exhibits symmetry we can use it to our advantage. Instead of choosing the initial vector at random we may construct it by means of a function that belongs to the desired symmetry class. As a result, we will obtain the eigenfunction of such a symmetry class with the smallest eigenvalue. For example, in order to obtain the first three eigenvalues of the Hamiltonian operator (10) shown in table 1, we chose the initial functions

\[
F_1(x_1, x_2, x_3, x_4) = e^{-x_1^2 - x_2^2 - x_3^2 - x_4^2},
\]

\[
F_2(x_1, x_2, x_3, x_4) = x_i e^{-x_1^2 - x_2^2 - x_3^2 - x_4^2}, \quad i = 1, 2, 3, 4,
\]

\[
F_3(x_1, x_2, x_3, x_4) = (x_1 + x_2 + x_3 + x_4) e^{-x_1^2 - x_2^2 - x_3^2 - x_4^2}.
\]

Figure 3 shows the rate of convergence of the approximate eigenvalues in terms of the number of iterations of the algorithm. The solid line corresponds to a random initial vector and the other curves are given by initial vectors obtained from the functions indicated above. On choosing a random initial vector the algorithm converges towards the ground state after 80 iterations. On the other hand, the use of the symmetry-adapted functions enables us to achieve the same accuracy with noticeably fewer iterations. Comparison of execution times is meaningless unless all the calculations are carried out under exactly the same conditions. As a reference we mention that the 74 iterations corresponding to the solid line took \( Δt = 8.69 \) s on a PC with a 1.83 GHz Intel processor Core Duo and 3 Gb of RAM memory. Another relevant piece of information is that we used Mathematica 7 in all our calculations. Obviously, the other curves based on the symmetry-adapted functions took less time.

Some time ago, Tymczak and Wang [37] calculated the eigenvalues of a three-dimensional harmonic oscillator (\( D = 3 \), \( ν_{ij} = 0 \)) by means of different basis sets of wavelets. In table 2, we compare our results, obtained with grids of different sizes and the scale parameter \( L \) optimized as discussed above, with those of table I of [37]. Table 2 shows that our results are considerably more precise than their most accurate ones given by wavelets \( D_{14} \).

4. Two coupled anharmonic oscillators

In this section, we apply our approach to two coupled anharmonic oscillators considered earlier by other authors.
4.1. The Pullen–Edmonds Hamiltonian

Our first example of the two-dimensional anharmonic oscillator is the so-called Pullen–Edmonds Hamiltonian [15, 16]

\[
\hat{H} = -\frac{1}{2} \nabla^2 + \frac{1}{2} \left( \kappa x^2 + y^2 \right). \tag{18}
\]

Proceeding as indicated above, we obtain the eigenvalues of the Hamiltonian matrix, and table 3 shows the first four of them for \( \kappa = 1 \). We clearly appreciate that the variational eigenvalues converge reasonably fast as \( N \) increases.

Some time ago, Fessatidis et al [11] chose the Pullens–Edmonds Hamiltonian (18) with \( \kappa = 1 \) to test their proposed variational approach. The results obtained by those authors for the ground state, reported in their table I, clearly converge to a limit that is greater than the one obtained here by means of the LSF. The reason for the erroneous results of Fessatidis et al [11] lies not in the method used to solve the problem, but in the fact that the authors have resorted to an unsuitable spherically symmetric basis set \( \{ \phi_n(r) \} \), where \( r = \sqrt{x^2 + y^2} \). Since the eigenfunctions of \( \hat{H} \) depend on two variables, for example \( \psi_n(x, y) \) or \( \psi_n(r, \phi) \), \( x = r \cos \phi, y = r \sin \phi \), the spherical-symmetric basis generated by Fessatidis et al [11] is not complete and their eigenvalues do not converge to those of the Hamiltonian operator (18). In fact, the authors obtained the eigenvalues of an effective central-field Hamiltonian operator in which the average

\[
\frac{1}{2\pi} \int_0^{2\pi} \psi_n^2 \, d\phi = \frac{r^4}{8} \tag{19}
\]

substitutes the anisotropic part of the potential in equation (18):

\[
\hat{H} = -\frac{1}{2} \nabla^2 + \frac{1}{2} r^2 + \frac{\kappa}{8} r^4. \tag{20}
\]

As a further confirmation of this assumption, we applied the most accurate Riccati–Padé method [38] and estimated that the ground-state eigenvalue of this operator for \( \kappa = 1 \) is \( E_0 = 1.179 \, 071 \, 199 \, 615 \, 515 \, 2844 \), which is an improvement on the result reported by Fessatidis et al [11], \( E_0 = 1.179 \, 071 \, 1965 \).

Arias de Saavedra and Buendia [19] and more recently Killingbeck and Jolicard [23] studied a slightly modified version of the Pullen–Edmonds Hamiltonian operator:

\[
\hat{H} = p_x^2 + p_y^2 + x^2 + y^2 + \lambda x^2 y^2. \tag{21}
\]

In order to compare our results with theirs, we have calculated the ground-state eigenvalue of this operator for several values of the coupling parameter \( \lambda \), and table 4 shows our results for \( N = 100 \) and 120. As discussed elsewhere,

we can improve the LSF calculations by means of adjustable parameters, and coordinate rotations enable us to introduce variational rotation angles [39]. We also determine their optimum values by means of the PMS as discussed in subsequent sections. In the case of the Pullen–Edmonds Hamiltonian, we find that a coordinate rotation by an angle \( \theta = \pi/4 \) is close to the optimal, so that the resulting Hamiltonian operator reads

\[
\hat{H} = p_x^2 + p_y^2 + x^2 + y^2 + \frac{\lambda}{4} \left( x^2 - y^2 \right)^2. \tag{22}
\]

Both operators are connected by a unitary transformation and have exactly the same eigenvalues. However, the rate of convergence of the present LSF approach is greater for the Hamiltonian operator in equation (22) as shown in table 4. In this case, our results compare favourably with those reported by Arias de Saavedra and Buendia [19] and Killingbeck and Jolicard [23].

We may try an intuitive justification of why the LSF is more efficient for the rotated Hamiltonian operator (22) than for the unrotated one (21). The shaded area in figure 4 shows the classically allowed region for the unrotated Hamiltonian with \( \lambda = 10 \) and energy \( E = 4 \). The two squares show the minimal discretization areas that fully enclose the classically allowed region. The rotated internal one fits the classically allowed region more tightly and appears to be more efficient for discretization because it leaves less 'wasted' area. Note that a similar argument for the phase-space region has already been provided by Fattal et al [24]. Clearly, the minimization of the trace discussed above provides a simple and efficient criterion even for higher dimensional problems where geometrical considerations may be more difficult.

4.2. Quartic oscillators

Our second example of two coupled anharmonic oscillators is given by

\[
\hat{H} = \frac{p_1^2}{2m_1} + \frac{1}{2} m_1 \omega_1^2 x_1^2 + \frac{p_2^2}{2m_2} + \frac{1}{2} m_2 \omega_2^2 x_2^2 + \lambda \left( c_{40} x_1^4 + c_{04} y_1^4 + c_{22} x_1^2 y_2^2 \right) \tag{23}
\]

Incidentally, the reader may verify that \( \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dV (x \cos \theta - y \sin \theta, x \sin \theta + y \cos \theta) \) does not depend on \( \theta \), which clearly shows that all the grids are equivalent in the continuum limit.
shows the present results for the first three
have been obtained (25) (26)
the symmetry of the problem as discussed above. For example,
require \( \Delta t = t \)
and/or \( \beta \) and \( \gamma \) are chosen to minimize it. Note that
and several values of \( \lambda \). Here we restrict ourselves to the most unfavourable case \( \lambda = 10^6 \).
We have applied our collocation method to this problem following three approaches. The first approach is the one followed so far, which uses the minimization of the trace of the Hamiltonian matrix to generate the optimal scale \( L \) for a given grid. The results in table 6 have been obtained in this straightforward way that does not take into account the anisotropy of the potential. In the second approach, we take into account that anisotropy by simply rescaling the \( y \) and \( z \) coordinates, \( y \rightarrow \beta y \) and \( z \rightarrow \gamma z \), with two adjustable parameters \( \beta \) and \( \gamma \). Thus, the resulting eigenvalue equation becomes

\[
\frac{1}{2} \left[ \frac{\partial^2}{\partial x^2} + \beta^2 \frac{\partial^2}{\partial y^2} + \gamma^2 \frac{\partial^2}{\partial z^2} \right] \psi(x, y/\beta, z/\gamma) = (E - V(x, y/\beta, z/\gamma)) \psi(x, y/\beta, z/\gamma).
\]

and the trace of the Hamiltonian matrix explicitly depends upon \( \beta \), \( \gamma \) and \( L \), which are chosen to minimize it. Note that this approach is equivalent to choosing LSF with different length scales on the three axes, say \( L_x \), \( L_y \) and \( L_z \). Table 7 shows the convergence of the eigenvalues obtained in this way as the matrix dimension increases.

The third approach consists of introducing additional adjustable parameters by means of a coordinate rotation of the form

\[
x' = x \cos \theta_1 \cos \theta_2 - y \sin \theta_1 - z \cos \theta_1 \sin \theta_2,
\]

\[
y' = x \sin \theta_1 \cos \theta_2 + y \cos \theta_1 - z \sin \theta_1 \sin \theta_2,
\]

\[
z' = x \sin \theta_2 + z \cos \theta_2,
\]
so that the trace of the Hamiltonian matrix now depends on $L$, $\beta$, $\gamma$, $\theta_1$ and $\theta_2$. Only the potential part of the matrix will depend on the rotation angles because the kinetic energy is invariant under such a transformation. Note that this approach is similar to the one discussed above for the Pullen–Edmonds Hamiltonian. Table 8 shows the convergence of the eigenvalues obtained in this way as the matrix dimension increases.

Table 9 shows the values of the optimal parameters for the three methods outlined above. Elsewhere we outline some features of the variational method and suggest that the LSF approach exhibits variational behaviour that is different from that of a basis set of harmonic-oscillator eigenfunctions [39].

5.2. Sextic oscillator

Our second example of three-dimensional anharmonic oscillator is given by the Hamiltonian operator

$$H = \frac{1}{2} \left( p_1^2 + p_2^2 + p_3^2 \right) + \frac{1}{2} \left( x_1^2 + x_2^2 + x_3^2 \right) + \frac{1}{2} \left( x_1^4 + x_2^4 + x_3^4 \right) \quad \text{(27)}$$

studied by Braun et al [12] and Chung and Chew [10]. Table 10 shows our numerical results for several matrix dimensions and a variationally optimized grid scale $L$. We show the eigenvalues obtained by Braun et al [12] and Chung and Chew [10] for comparison. The last row of table 10 shows the most accurate eigenvalues obtained by Chung and Chew [10] with a matrix of size $17^3 \times 17^3$.

6. Four coupled sextic oscillator

As an example of the four-dimensional anharmonic oscillator we choose the model studied by Kaluza [13] and Chung and Chew [10]:

$$H = \frac{1}{2} \left( p_1^2 + p_2^2 + p_3^2 + p_4^2 \right) + \frac{1}{2} \left( x_1^2 + x_2^2 + x_3^2 + x_4^2 \right) + \frac{1}{2} \left( x_1^4 + x_2^4 + x_3^4 + x_4^4 \right)$$

Table 11 compares the present results with the ones obtained by those authors and we note that our eigenvalues are more accurate than those of Chung and Chew [10] even for matrices of size as small as $9^4 \times 9^4$.

7. Conclusions

In this paper, we have extended the variational collocation approach developed earlier in one dimension [25] to the solution of the Schrödinger equation for systems of coupled oscillators or single oscillators in more than one dimension. We have applied our method to several examples previously considered in the literature and obtained remarkably accurate results for all of them. In particular, we have shown how to improve the rate of convergence of our approach by means of nonlinear variational parameters. We underline some of the virtues of our approach: its application is straightforward and not limited to polynomial potentials; the construction
of the Hamiltonian matrix does not involve the numerical calculation of integrals; one obtains its kinetic part for a given grid once and for all and stores it for applications to problems that differ in the potential-energy function; the potential part of the Hamiltonian matrix is diagonal; the Hamiltonian matrix is an analytic function of the variational parameters, which greatly facilitates the numerical determination of the minimum of its trace.

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