JOURNAL OF COMPUTATIONAL PHYSICS **126,** 315–327 (1996)
ARTICLE NO. 0140

An Efficient Chebyshev–Lanczos Method for Obtaining Eigensolutions of the Schrödinger Equation on a Grid

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Received July 28, 1995; revised December 4, 1995

A grid method for obtaining eigensolutions of bound systems is presented. In this, the block–Lanczos method is applied to a Chebyshev approximation of $\exp(-H/\Delta)$, where Δ is the range of eigenvalues we are interested in. With this choice a preferential convergence of the eigenvectors corresponding to low-lying eigenvalues of H is achieved. The method is used to solve a variety of one-, two-, and three-dimensional problems. To apply the kinetic energy operator we use the fast sine transform instead of the fast Fourier transform, thus fullfilling, *a priori*, the box boundary conditions. We further extend the Chebyshev approximation to treat general functions of matrices, thus allowing its application to cases for which no analytical expressions of the expansion coefficients are available.

I. INTRODUCTION

Grid methods have been extensively used in the past to solve the time-dependent Schrödinger equation (TDSE),

$$\frac{\partial \Psi(\mathbf{r}, t)}{\partial t} = -iH\Psi(\mathbf{r}, t), \tag{1}$$

for various quantum systems in atomic and molecular physics [1, 2]. The solution of the TDSE contains all the dynamics of the system and therefore a wide range of phenomena can be studied, such as the diffractive scattering from crystalline surfaces, atom scattering from imperfect and disordered surfaces, rotationally and vibrationally inelastic molecule-surface scattering, excitation of surface phonons and of electron–hole pairs, etc. Moreover, the grid methods have also proved useful in treating the problems of localization of waves, particles moving in almost periodic potentials, phonons, and enhanced back-scattering of light by random media, etc. These studies involve the propagation of wave packets forward in time.

Apart from the continuum, the grid methods have also been employed in bound state calculations, where the spectrum of the Hamiltonian can be obtained from the solution of the TDSE. The problem usually encountered is the diagonalization of the Hamiltonian H in (1). Since this in practice cannot be done, it is impossible to compute the action of the propagator e^{-itH} on an arbitrary wave function [2] and, thus, the time-evolution is accomplished using various approximations to the exponential. We mention here the Crank–Nicolson scheme [3–5] and the Kosloff and Tal-Ezer method [6]. For a detailed discussion we refer the reader to the review article of de Raedt [2]. The existing methods, although simple to use, can be quite CPU-time intensive, especially in calculating a large number of bound states in more than one dimension.

To circumvent the need for long propagation times, Neuhauser proposed the so-called filter-diagonalization method [7] to obtain bound-state eigenfunctions in any arbitrary range of energies. This is achieved by propagating forward in time an arbitrary initial wave packet under the influence of the Hamiltonian H to obtain the wave function $\psi(\mathbf{x}, t) \equiv \exp(-iHt)\psi(\mathbf{x})$. A small set of approximate eigenstates within a desired energy range is then prepared, which is used as a small basis for time independent extraction (by diagonalization) of the sought eigenstates. In a recent article, a more elaborate description and extension of the method has been given by Wall and Neuhauser [8]. Yet another interesting method concerning the eigenvalue problem for large matrices has been proposed by Wyatt [9]. In this, the Green function filter is employed in the Lanczos algorithm to obtain eigenvalues in a specific range. More details and references to similar methods can be found in the aforementioned references.

In this work an alternative method for obtaining eigenvalues and eigenfunctions is presented. The method employs the block–Lanczos method with selective orthogonalization [10] to a Chebyshev approximation of $\exp(-H/\Delta)$, where Δ is the range of eigenvalues we are interested in. With this choice, a preferential convergence for the eigenvectors corresponding to the low-lying eigenvalues of H can be achieved. Unlike the method of Neu-

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0021-9991/96 $18.00

hauser we do not require very accurate propagation in time since we only use it to facilitate convergence of the block–Lanczos method for low-lying eigenvalues where as in the filter-diagonalization method the accuracy of the propagation is essential for obtaining the eigenvalues.

In the following section the grid, Chebyshev, and Lanczos methods are briefly reviewed together with the proposed modifications. In Section III, we apply the method to one-, two-, and three-dimensional examples and compare the results to those of competing methods. Finally, in Section IV a summary of our conclusions is given.

II. THE GRID METHOD

We are concerned with the determination of the eigenfunctions and eigenvalues of the ν-dimensional Hamiltonian

$$H = T + V = -\frac{\hbar^2}{2m}\sum_{i=1}^{\nu}\frac{\partial^2}{\partial x_i^2} + V(x_1, ..., x_\nu), \tag{2}$$

where x_i are the coordinates describing the system and V is the potential energy. The grid method in ν dimensions discretizes the wave function Ψ in the ν-dimensional box,

$$[a_1, b_1] \times [a_2, b_2] \times \cdots \times [a_\nu, b_\nu], \tag{3}$$

by choosing n_i equidistant grid-points in each dimension

$$x_k^{(i)} = a_i + \frac{k}{n_i}(b_i - a_i), \quad k = 0, ..., n_i - 1. \tag{4}$$

The wavefunction Ψ is thus described by its $N := n_1 n_2 \cdots n_\nu$ values on the grid. The application of the Hamiltonian operator on the wave function in coordinate space is written

$$\langle r|H|\Psi\rangle = \langle r|T|\Psi\rangle + \langle r|V|\Psi\rangle \tag{5}$$

with

$$\langle r|V|\Psi\rangle = V(r)\Psi(r) \tag{6}$$

and

$$\langle r|T|\Psi\rangle = \frac{\hbar^2}{2m}\int dk \sum_i k_i^2 \frac{e^{-i\mathbf{r}\cdot\mathbf{k}}}{\sqrt{2\pi}}\Phi(k). \tag{7}$$

Here $|r\rangle = |x_1 x_2 \cdots x_\nu\rangle$, $|k\rangle = |k_1 k_2 \cdots k_\nu\rangle$, and $dk = dk_1\, dk_2 \cdots dk_\nu$ while $\Phi(k)$ is the Fourier transform of $\Psi(r)$. Thus, in order to apply the kinetic energy operator on $\Psi(r)$, one first Fourier-transforms it to $\Phi(k)$, applies the kinetic energy operator, and then uses the inverse Fourier transform to return to the **r**-space. The potential energy V is diagonal in **r**-space and the kinetic energy T is diagonal in momentum space (**k**-space). Therefore, the fast Fourier transform (FFT) is usually employed for the application of the kinetic energy operator to the wave function. This requires each n_i to be a power of 2 [11].

For bound states, the boundary condition is that Ψ vanishes on the boundaries of the box. In previous implementations of the grid method [6] the FFT was used, which is not well suited to this boundary condition, and then one has to resort to tricks such as the introduction of reflecting walls (very large potential values at the boundary). In this work we employ the fast sine transform (FST) [11], which *a priori* satisfies the box boundary conditions. To introduce the FST we first recall the definition of the sine transform,

$$\Phi_k = \sum_{j=0}^{N-1}\Psi_j \sin(\pi jk/N), \quad k = 0, ..., N-1, \tag{8}$$

where Ψ_j are the values of the wavefunction at the equidistant grid-points with $\Psi_0 = 0$ by default. Then the FST is defined by applying the FFT to an auxiliary array y_j,

$$\begin{aligned} y_0 &= 0 \\ y_j &= \sin(j\pi/N)(\Psi_j + \Psi_{N-j}) \\ &\quad + \tfrac{1}{2}(\Psi_j - \Psi_{N-j}), \quad j = 1, ..., N-1, \end{aligned} \tag{9}$$

yielding the result

$$Y_k = \sum_{j=0}^{N-1} e^{2\pi ijk/N} y_j. \tag{10}$$

The sine transform of the original array is then obtained via

$$\begin{aligned} \Phi_{2k} &= \mathrm{Im}\, Y_k \\ \Phi_{2k+1} &= \Phi_{2k-1} + \mathrm{Re}\, Y_k \\ \Phi_1 &= \tfrac{1}{2}\,\mathrm{Re}\, Y_0 \end{aligned} \tag{11}$$

A method frequently used to determine the low-lying eigenvalues of a system is the relaxation approach [6] which can be computationally demanding. In this work, we propose an efficient alternative method, namely, we apply the block–Lanczos method to a Chebyshev approximation of $\exp(-H/\Delta)$. In this way a tridiagonal representation of the Hamiltonian is obtained and, hence, the calculation of the eigenvalues is greatly simplified. In order to describe our method we first outline the Chebyshev and Lanczos methods.

A. The Chebyshev Expansion

The Chebyshev expansion method for functions of matrices [2, 12] has been used in the past to propagate the

wave function in time [1] or in conjunction to relaxation methods [6]. In this, a function $f(y)$, with $y \in [a, b]$, is expanded in terms of the Chebyshev polynomials of the first kind $T_i(x)$,

$$f(y) = \sum_{i=0}^{\infty} c_i T_i\left(\frac{2y - (b+a)}{b-a}\right), \tag{12}$$

with the expansion coefficients being given by

$$c_i = \frac{2 - \delta_{i,0}}{\pi} \int_{-1}^{+1} \frac{T_i(x) f\left(\frac{b-a}{2}x + \frac{b+a}{2}\right)}{\sqrt{1-x^2}}\, dx. \tag{13}$$

In the above expression (12) one can substitute for y a symmetric $N \times N$ matrix $\mathbf{A}$, provided its eigenvalues fall in the range $[a, b]$. The corresponding Chebyshev expansion is

$$f(\mathbf{A}) = \sum_{i=0} c_i T_i(\mathbf{B}) \tag{14}$$

with

$$\mathbf{B} = \frac{2}{b-a}\mathbf{A} - \frac{b+a}{b-a}\mathbf{I}, \tag{15}$$

where $\mathbf{I}$ is the unit matrix. Such an expansion has been employed by Kosloff and Tal-Ezer [6] for the exponential $e^{-H\tau}$, with the expansion coefficients expressed in terms of modified Bessel functions. Since analytical expressions cannot be obtained for a general function we shall present in Section C a numerical alternative.

B. The Lanczos Method

The Lanczos method [10, 13, 14] has been widely used for computing a few of the extreme eigenvalues and the corresponding eigenvectors of large symmetric matrices [15]. The method has also been employed in the framework of the discrete variable representation (DVR) [16], which can be considered as a generalization of the grid method. More recently, the so-called analytical Lanczos method has been applied, using the symbolic manipulation package Mathematica, to the sextic anharmonic oscillator and to two, three, and four coupled anharmonic oscillators [17]. In this work, the block–Lanczos method is used since the matrix enters only through its application to a vector and, therefore, it allows us to exploit the FST-representation for the kinetic energy term, while standard eigenvalue methods require the elements of the matrix to be explicitly known.

Let $\mathbf{A}$ be a symmetric $N \times N$ matrix. If we consider an eigenvalue λ_i of $\mathbf{A}$ at the upper end of the spectrum ($i \sim N$) the eigenvalue estimate $\lambda_i^{(n)}$, obtained after n steps of the Lanczos method satisfies [18]

$$\lambda_i - \lambda_i^{(n)} \le (\lambda_i - \lambda_1)\left(\frac{K_i^{(n)}}{T_{n+i-N}(\gamma_i)} \tan[\theta(\mathbf{y_i}, \mathbf{x}_0)]\right)^2, \tag{16}$$

where

$$K_i^{(n)} = \prod_{j=1}^{N-i} \frac{\lambda_{N-j}^{(n)} - \lambda_1}{\lambda_{N-j}^{(n)} - \lambda_i} \tag{17}$$

and

$$\gamma_i = 1 + 2\frac{\lambda_i - \lambda_{i-1}}{\lambda_{i-1} - \lambda_1}. \tag{18}$$

The $\theta(\mathbf{y_i}, \mathbf{x_0})$ is the angle between the starting vector $\mathbf{x_0}$ of the Lanczos method and the eigenvector $\mathbf{y_i}$ while $T_n(x)$ is the nth-order Chebyshev polynomial. An analogous relation holds for the lower end of the spectrum ($i \sim 1$). In either case the rate of convergence for the eigenvalue λ_i is bounded by

$$\tau_i = (\gamma_i + \sqrt{\gamma_i^2 - 1})^2, \tag{19}$$

as can be seen by substituting the following expression in Eq. (16)

$$T_k(x) = (x + \sqrt{x^2-1})^k + (x - \sqrt{x^2-1})^k. \tag{20}$$

In the block-version of the Lanczos method, where a system of r linear independent vectors is used, similar convergence criteria can be obtained by replacing γ_i with

$$\gamma_i' = 1 + 2\frac{\lambda_i - \lambda_{i-r}}{\lambda_{i-r} - \lambda_1}. \tag{21}$$

Direct application of the block–Lanczos method to the grid representation $\mathbf{H}_g$ of the Hamiltonian will, however, be inefficient for obtaining the low-lying eigenvalues. This is due to the fact that the gaps at the upper end of the spectrum are typically much larger than the gaps between the low-lying eigenvalues that we are interested in. This results in a slow convergence for the lower eigenvalues and large storage requirements, since all the Lanczos vectors generated have to be retained. This problem is clearly demonstrated by the ground state calculation performed for the ozone (O_3) molecule by Le Quéré and Leforestier [16], where more than 100 iterations were needed to obtain a reliable value for the ground state energy.

C. The Chebyshev–Lanczos Method

In order to enhance the convergence for the low-lying eigenvalues, we apply the Lanczos method to a Chebyshev approximation of $\exp(-\mathbf{H}_g/\Delta)$, where Δ is the range of eigenvalues we are interested in. The eigenvalues of $\exp(-\mathbf{H}_g/\Delta)$ are given by $\mu_i = \exp(-\lambda_i/\Delta)$. The μ_i corresponding to λ_i within a range of the order of Δ from λ_1 will have the largest gaps $\mu_{i+1} - \mu_i$ and therefore will be the first to converge (see Eq. (16)), while the eigenvalues at the upper end of the spectrum of H are mapped to the vicinity of zero and do not interfere with the calculation.

For the preferential convergence of the μ_i, corresponding to the low-lying eigenvalues of H, the accuracy of the Chebyshev approximation is however not crucial, since the exact behaviour of the approximation for eigenvalues outside the range of interest is not important, as long as those μ_i are sufficiently close to zero. It is therefore sufficient to approximate the exponential with a tolerance δ of the order of $\exp[-(\lambda_1/\Delta + O(1))]$.

For practical applications we use the block–Lanczos method with selective orthogonalization (LASO) [10] to prevent the appearance of multiple copies of eigenvectors. To obtain the original eigenvalues from those determined for the Chebyshev approximation we simply calculate the expectation values of $\mathbf{H}_g$ with respect to the eigenvectors via

$$E_i = \langle \mathbf{y}_i | H_g | \mathbf{y}_i \rangle, \tag{22}$$

i.e., using the fact that a Taylor expandable function of a matrix has the same eigenvectors as the matrix itself.

In the work done sofar, the Chebyshev approximation was only applied to the exponential, for which closed expressions for the coefficients of the Chebyshev expansion exist. To have a method that works for any sufficiently smooth function $g(x)$ we modified the above procedure by determining the coefficients d_i of the Chebyshev interpolating expansion of order M,

$$g(x_k) = \sum_{i=0}^{M} d_i T_i(x_k), \tag{23}$$

which is exact at all the $M + 1$ zeros x_k of $T_{M+1}(x)$ and truncated the expansion at a suitable value $m < M$. Assuming that the interpolation of order M is virtually exact, and using the property that the Chebyshev polynomials are bounded by unity, the truncation order m can be determined for a specified tolerance δ by requiring

$$\sum_{i=m+1}^{M} |d_i| < \delta. \tag{24}$$

The coefficients d_i are obtained via the discrete orthogonality relations for the Chebyshev polynomials [11]

$$d_0^{(M)} = \frac{1}{M+1} \sum_{k=1}^{M+1} g(x_k) \tag{25}$$

and

$$d_i^{(M)} = \frac{2}{M+1} \sum_{k=1}^{M+1} g(x_k) \cos\left(\frac{\pi i (k - \frac{1}{2})}{M+1}\right), \quad 0 \le i \le M, \tag{26}$$

where

$$x_k = \cos\left(\frac{\pi (k - \frac{1}{2})}{M+1}\right). \tag{27}$$

Thus the integration in Eq. (13) has been replaced by a summation involving cosines only.

III. NUMERICAL EXAMPLES

In the following, we shall apply our method to one-, two-, and three-dimensional cases and compare our results with those of competing methods.

A. The One-Dimensional Case

1. *The Malfliet–Tjon Potential*

The Malfliet–Tjon I + III nucleon–nucleon potential [19] is widely used in bound state and scattering calculations in the field of few-nucleon physics. The potential for the $^3S_1$-channel is given by

$$V(x) = (1438.72 \exp(-3.11x)/x - 626.885 \exp(-1.55x)/x), \tag{28}$$

where the units are in the MeV-fm system.

Starting with a random vector, using a 1024-grid in the interval $[0, 32]$, a range parameter of $\Delta = 20$, and a Chebyshev tolerance $\delta = 0.1$ we obtained a bound state energy of -2.2309 MeV in very good agreement with the result of -2.2306 MeV by Payne [20] which was obtained by using the collocation method with Hermite splines.

2. *The Morse Oscillator*

The Morse oscillator is a tricky one-dimensional problem, whose closely spaced eigenvalues require a long propagation interval τ in the relaxation method of Kosloff [6].

TABLE I

The 25 Lowest Eigenvalues of the Morse Oscillator for the I_2-Molecule

ν	analytical [21]	present	difference
0	.286171979 10^{-3}	.286171969 10^{-3}	-.10 10^{-10}
1	.852996624 10^{-3}	.852996593 10^{-3}	-.30 10^{-10}
2	.141246218 10^{-2}	.141246213 10^{-2}	-.50 10^{-10}
3	.196456866 10^{-2}	.196456859 10^{-2}	-.70 10^{-10}
4	.250931606 10^{-2}	.250931597 10^{-2}	-.89 10^{-10}
5	.304670436 10^{-2}	.304670426 10^{-2}	-.11 10^{-9}
6	.357673359 10^{-2}	.357673346 10^{-2}	-.13 10^{-9}
7	.409940373 10^{-2}	.409940359 10^{-2}	-.15 10^{-9}
8	.461471479 10^{-2}	.461471463 10^{-2}	-.16 10^{-9}
9	.512266677 10^{-2}	.512266658 10^{-2}	-.18 10^{-9}
10	.562325966 10^{-2}	.562325946 10^{-2}	-.20 10^{-9}
11	.611649346 10^{-2}	.611649325 10^{-2}	-.22 10^{-9}
12	.660236819 10^{-2}	.660236795 10^{-2}	-.23 10^{-9}
13	.708088382 10^{-2}	.708088357 10^{-2}	-.25 10^{-9}
14	.755204038 10^{-2}	.755204011 10^{-2}	-.27 10^{-9}
15	.801583785 10^{-2}	.801583757 10^{-2}	-.28 10^{-9}
16	.847227624 10^{-2}	.847227594 10^{-2}	-.30 10^{-9}
17	.892135554 10^{-2}	.892135523 10^{-2}	-.32 10^{-9}
18	.936307576 10^{-2}	.936307543 10^{-2}	-.33 10^{-9}
19	.979743690 10^{-2}	.979743655 10^{-2}	-.35 10^{-9}
20	.102244390 10^{-1}	.102244386 10^{-1}	-.36 10^{-9}
21	.106440819 10^{-1}	.106440815 10^{-1}	-.38 10^{-9}
22	.110563658 10^{-1}	.110563654 10^{-1}	-.39 10^{-9}
23	.114612906 10^{-1}	.114612902 10^{-1}	-.41 10^{-9}
24	.118588563 10^{-1}	.118588559 10^{-1}	-.42 10^{-9}

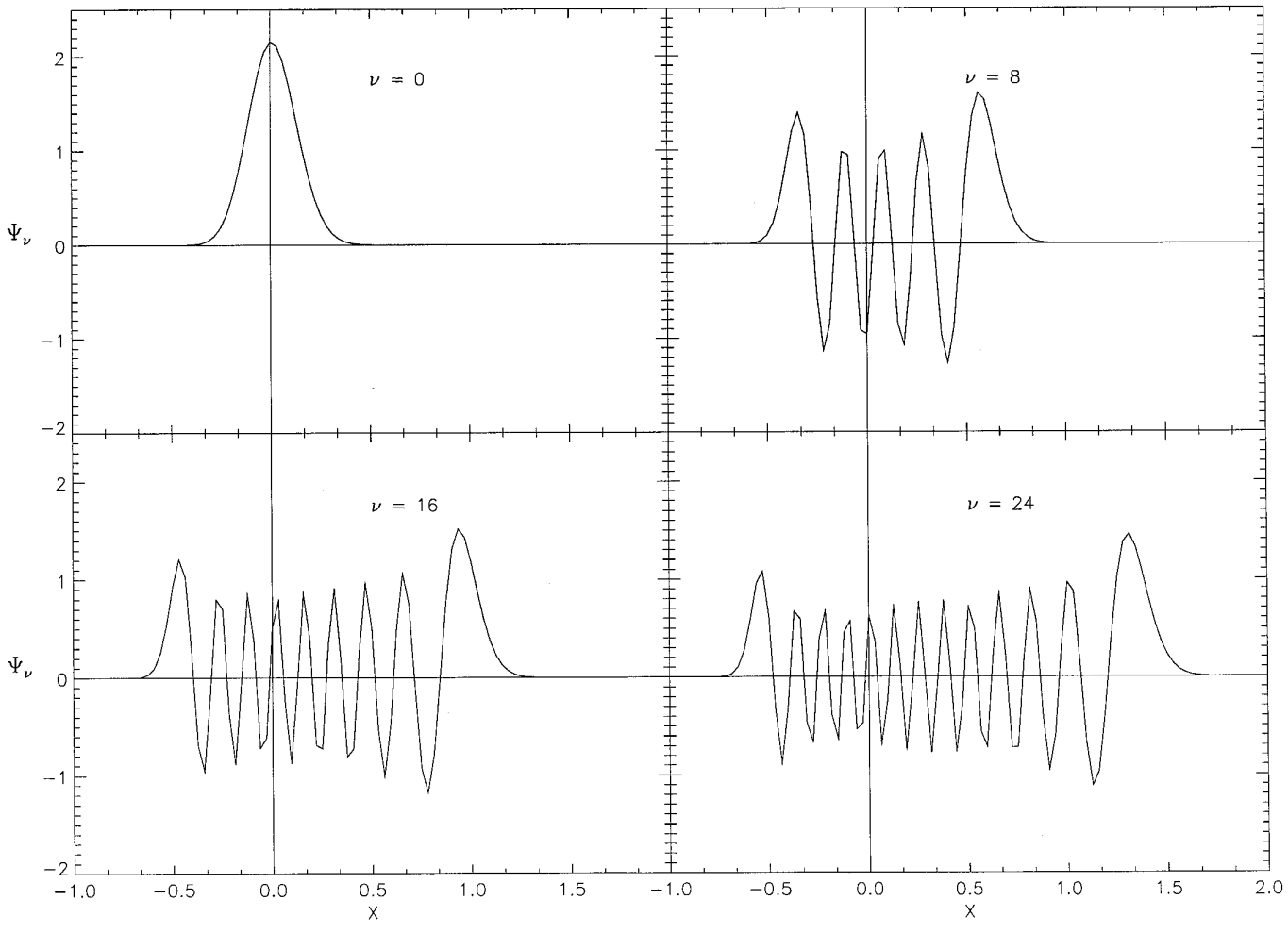

FIG. 1. The wavefunctions obtained for the Morse oscillator for $\nu = 0$, 8, 16, and 24.

We consider the Morse potential for the I_2-molecule which is given by

$$V(x) = D[\exp(-2\alpha x) - 2\exp(-\alpha x)] + D \qquad (29)$$

with $D = 0.0224$ a.u., $\alpha = 0.9374$ a.u., and a reduced mass of $\mu = 119406$ a.u. The D has been added to shift the minimum of the potential to zero. The analytical expression for the eigenvalues is [21]

$$E_\nu = \left(\nu + \frac{1}{2} - \frac{1}{\zeta}\left[\nu + \frac{1}{2}\right]^2\right) 5.741837286 \times 10^{-4}\ \text{a.u.}, \quad \nu \geq 0, \qquad (30)$$

with $\zeta = 156.047612535$. The eigenfunctions Ψ_ν can be expressed in terms of Kummer functions [21], or, alternatively, generalized Laguerre polynomials [22],

$$\Psi_\nu = N_\nu y^{p/2} \exp(-\tfrac{1}{2}y) L_\nu^p(y), \qquad (31)$$

where $y = \zeta \exp(-\alpha x)$, $p = \zeta - 2\nu - 1$ and with the normalization factor

$$N_\nu = \left\{\frac{\Gamma(p)}{\alpha}\sum_{\lambda=0}^{\nu}(-1)^\lambda \binom{-p}{\lambda}\right\}^{-1/2}. \qquad (32)$$

The latter can be obtained through manipulation of the generating function of the generalized Laguerre polynomials [22].

We used the block-version of the Lanczos method with a blocksize of $r = 8$, starting with random vectors. The results of our calculations are given in Table I. We used 128 grid points in the interval $[-1, 3]$. The range parameter was chosen as $\Delta = 0.02$ and the Chebyshev tolerance as $\delta = 0.1$. The calculation of the 25 lowest eigenvalues took

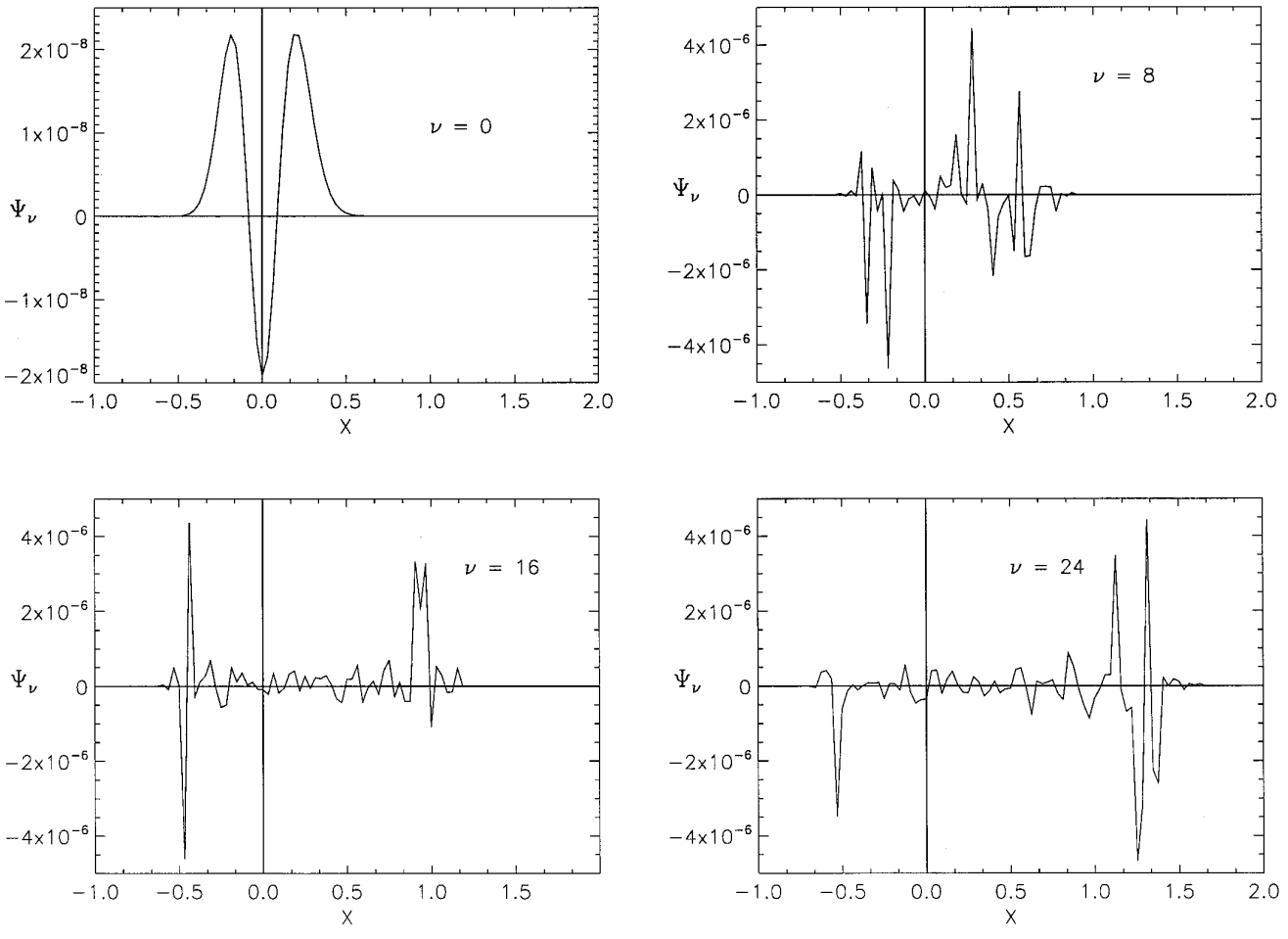

FIG. 2. The difference between the numerical and the analytical wavefunctions obtained for the Morse oscillator for $\nu = 0$, 8, 16, and 24.

8.63 CPU-seconds on an IBM-RISC 6000/340 workstation. It is seen that the accuracy achieved is between 6 to 8 digits. A higher accuracy can be achieved by increasing the number of grid points.

To convey an impression of the eigenfunctions and to demonstrate the economy of the method, we have plotted in Fig. 1 the resulting eigenfunctions for $\nu = 0$, 8, 16, and 24. Although there are only about four grid points per period for the $\nu = 24$ eigenfunction, we still obtain the eigenvalue with a 7-figure accuracy.

To compare the numerical eigenfunctions with the analytical ones, we normalized them according to

$$h_x \sum_{i=0}^{127} \Psi_\nu^{\text{num}}(x_i)^2 = 1, \tag{33}$$

corresponding to

$$\int_a^b \Psi_\nu^{\text{exact}}(x)^2\, dx = 1$$

for $N \to \infty$.

In Fig. 2 we show the differences between the numerical and analytical eigenfunctions. It is seen that the difference is less than 10^{-5} for all cases. Another measure of the difference is

$$e_\nu := \left(h_x \sum_{i=0}^{127} (\Psi_\nu^{\text{num}}(x_i) - \Psi_\nu^{\text{exact}}(x_i))^2 \right)^{1/2}. \tag{34}$$

The values thus obtained are smaller than 2×10^{-6} in all cases.

3. *The Anharmonic Sextic Oscillator*

The anharmonic sextic oscillator has been treated by Kaluza [17] in his paper on the analytical Lanczos method [17], where he gives eigenvalues that are very accurate for the 30 lowest states of even parity. Therefore, this provides a nontrivial case to test the performance and find what kind of accuracy our method can achieve.

The potential is given by

TABLE II

The 48 Lowest Eigenvalues of the Sextic Anharmonic Oscillator Corresponding to States of Even Parity

i	Kaluza [17]	present	difference
1	1.00000000000000000	1.00000000000000067	$.67\ 10^{-15}$
2	6.84840938290355083	6.84840938290355794	$.71\ 10^{-14}$
3	15.1189299862423532	15.1189299862423372	$-.16\ 10^{-13}$
4	25.0499485467589551	25.0499485467589658	$.11\ 10^{-13}$
5	36.3427162124129666	36.3427162124129453	$-.21\ 10^{-13}$
6	48.8188557894952027	48.8188557894951884	$-.14\ 10^{-13}$
7	62.3560289446043683	62.3560289446043612	$-.71\ 10^{-14}$
8	76.8635227337003784	76.8635227337003641	$-.14\ 10^{-13}$
9	92.2705755458715799	92.2705755458715799	0
10	108.519977962910005	108.519977962910033	$.28\ 10^{-13}$
11	125.564227036711259	125.564227036711188	$-.71\ 10^{-13}$
12	143.363055517025145	143.363055517025202	$.57\ 10^{-13}$
13	161.881761569277757	161.881761569277586	$-.17\ 10^{-12}$
14	181.090033347270861	181.090033347270776	$-.85\ 10^{-13}$
15	200.961094421342040	200.961094421341841	$-.20\ 10^{-12}$
16	221.471065493679532	221.471065493679419	$-.11\ 10^{-12}$
17	242.598476707488402	242.598476707488402	0
18	264.323887720018490	264.323887720018547	$.57\ 10^{-13}$
19	286.629586722251986	286.629586722251759	$-.23\ 10^{-12}$
20	309.499348483678148	309.499348483678261	$.11\ 10^{-12}$
21	332.918237321682568	332.918237321682454	$-.11\ 10^{-12}$
22	356.872444806447561	356.872444806447731	$.17\ 10^{-12}$
23	381.349154702387807	381.349154702387750	$-.57\ 10^{-13}$

$$V(x) = V_6(x) := \tfrac{1}{2}x^2 + 2x^4 + \tfrac{1}{2}x^6. \quad (35)$$

We used 512 grid points in the interval $[-8, 8]$. The range parameter was chosen as $\Delta = 1500$ and the Chebyshev tolerance as $\delta = 0.1$. Using a blocksize of $r = 6$ the algorithm required 178 CPU-seconds on an IBM-RISC 6000/340 workstation to obtain the 96 lowest eigenvalues. In Table II we show our results for the 48 lowest even-parity eigenstates for which Kaluza did his calculations. It is seen that up to the 35th even-parity eigenstate both methods agree to at least 14 figures.

TABLE II—*Continued*

24	406.336429536015828	406.336429536015714	-.11 10^{-12}
25	431.823114531145109	431.823114531145279	.17 10^{-12}
26	457.798755634855695	457.798755634856093	.40 10^{-12}
27	484.253529083002775	484.253529083002604	-.17 10^{-12}
28	511.178180496926018	511.178180496925734	-.28 10^{-12}
29	538.563971914420222	538.563971914419881	-.34 10^{-12}
30	566.402635473386795	566.402635473386567	-.23 10^{-12}
31	594.686332710882539	594.686332710882198	-.34 10^{-12}
32	623.407618631373566	623.407618631372770	-.80 10^{-12}
33	652.559409848831137	652.559409848831251	.11 10^{-12}
34	682.134956227356952	682.134956227357179	.23 10^{-12}
35	712.127815541317545	712.127815541318455	.91 10^{-12}
36	742.531830753778	742.531830753795475	.18 10^{-10}
37	773.34110957532	773.341109575325618	.56 10^{-11}
38	804.550006017	804.550006017276019	.28 10^{-9}
39	836.15310369	836.153103695176242	.52 10^{-8}
40	868.1452006	868.145200676664672	.77 10^{-7}
41	900.521295	900.521295691524529	.69 10^{-6}
42	933.276567	933.276575553427847	.56 10^{-5}
43	966.4064	966.406403658381464	.37 10^{-5}
44	999.906	999.906309444106569	.31 10^{-3}
45	1033.772	1033.77197871013732	-.21 10^{-4}
46	1068.00	1067.99924470990277	-.76 10^{-3}
47	1102.	1102.58407993753804	.58
48	1137.	1137.52258854123579	.52

B. The Two-Dimensional Case

1. *The Hénon–Heiles Potential*

The eigenvalues and eigenfunctions of the two-dimensional Hénon–Heiles potential have been treated by many authors in the study of anharmonically coupled oscillators (see Ref. [23] and references therein). This potential is given by

$$V(x,y)=\frac{1}{2}(x^2+y^2)+\frac{1}{4\sqrt{5}}x\left(y^2-\frac{1}{3}x^2\right). \quad (36)$$

TABLE III

The 32 Lowest Eigenvalues of the Hénon–Heiles System

(l,n)	Diagonalization [23]	present	Relaxation [6]
$(0,0)$	0.9986	0.998595	0.9986
$(\pm1,1)$	1.9901	1.990077	1.9901
		1.990077	1.9901
$(0,2)$	2.9562	2.956243	2.9562
$(\pm2,2)$	2.9853	2.985326	2.9853
		2.985326	2.9853
$(\pm1,3)$	3.9260	3.925964	3.9260
		3.925964	3.9260
$(\pm3,3)$	3.9824	3.982417	3.9820
	3.9858	3.985761	3.9836
$(0,4)$	4.8702	4.870144	4.8701
$(\pm2,4)$	4.8987	4.898644	4.8987
		4.898644	4.8988
$(\pm4,4)$	4.8963	4.986251	4.9860
		4.986251	4.9863
$(\pm1,5)$	5.8170	5.817019	5.8192
		5.817027	5.8193
$(\pm3,5)$	5.8670	5.867019	
	5.8815	5.881446	
$(\pm5,5)$	5.9913	5.991328	5.9912
		5.991328	
$(0,6)$	6.7379	6.737968	
$(\pm2,6)$	6.7649	6.764871	
		6.764955	
$(\pm4,6)$	6.8534	6.853436	
		6.853453	
$(\pm6,6)$	6.9989	6.998933	
	6.9994	6.999393	
$(\pm1,7)$	7.6595	7.659551	
		7.660248	
$(\pm3,7)$	7.6977	7.698226	
	7.7369	7.736915	

TABLE IV

The 13 Lowest Eigenvalues for a System of Two Coupled Sextic Anharmonic Oscillators (Kaluza only calculated the eigenstates with positive parity and exchange quantum numbers.)

i	Kaluza [17]	present	difference
1	1.992235763386565950	1.992235763386567	$0.10\ 10^{-14}$
2		4.305138454968618	
3		4.699323135716736	
4	6.895426376701	6.895426376506497	$-0.19\ 10^{-9}$
5		7.837870294086596	
6	7.9593012472	7.959301238963631	$-0.82\ 10^{-8}$
7		10.01652919760806	
8		10.58618828339855	
9		11.77888032499270	
10		11.80055533134312	
11		13.41554002288335	
12		14.20977578076531	
13	14.4805192	14.48196389062804	$0.14\ 10^{-2}$

We calculate the 32 lowest eigenvalues and eigenfunctions using a block size of $r = 4$, starting with random vectors. We worked with a 64×64 grid in $[-6, 6] \times [-6, 6]$, a range parameter of $\Delta = 10$ and a Chebyshev tolerance of $\delta = 0.1$. In Table III we show our results, along with those of the relaxation approach [6] and the diagonalization approach of Noid and Marcus [23]. Our results are in excellent agreement with those obtained through these methods. The calculation of all eigenfunctions and eigenvalues took 400 CPU-seconds on an IBM-RISC 6000/340 workstation.

2. *Two Coupled Anharmonic Oscillators*

The potential for two coupled anharmonic sextic oscillators reads [17]

$$V(x, y) = V_6(x) + V_6(y) + xy, \tag{37}$$

where V_6 is defined in Eq. (35) above. We have calculated the lowest 13 eigenstates and eigenvalues using a 64×64 grid in $[-4, 4] \times [-4, 4]$, a block size of $r = 4$, a range parameter $\Delta = 20$, and a Chebyshev tolerance of $\delta = 0.1$. This calculation took 187 CPU-seconds on an IBM-RISC 6000/340 workstation. Our results for the eigenvalues are shown in Table IV. The low-lying binding energies are in good agreement with the results of Kaluza.

C. The Three-Dimensional Case

1. *The Isotropic Three-Dimensional Harmonic Oscillator*

As a first example, we consider the isotropic three-dimensional harmonic oscillator with the potential

$$V(x, y, z) = \tfrac{1}{2}(x^2 + y^2 + z^2), \tag{38}$$

whose eigenvalues are given by

$$E_{n_x,n_y,n_z} = \tfrac{3}{2} + n_x + n_y + n_z. \tag{39}$$

The levels $E_n = \frac{3}{2} + n$ display a high degree of degeneracy that is given by

TABLE V

Eigenvalues of the Isotropic Three-Dimensional Harmonic Oscillator

$n = n_x + n_y + n_z$	n_d	exact	present
0	1	1.5	1.50000000000005862
1	3	2.5	2.50000000000007105
			2.50000000000008704
			2.50000000000009415
2	6	3.5	3.50000000000019673
			3.50000000000022515
			3.50000000000361355
			3.50000000000362821
			3.50000000000491029
			3.50000000000560085
3	10	4.5	4.50000000000151346
			4.50000000000370726
			4.50000000000375255
			4.50000000001024070
			4.50000000001243627
			4.50000000002715783
			4.50000000004485035
			4.50000000005976730
			4.50000000006838885
			4.50000000007554313

$$n_d = \frac{(n+1)(n+2)}{2}. \tag{40}$$

Using a $32 \times 32 \times 32$ grid in $[-6, 6] \times [-6, 6] \times [-6, 6]$ we obtained results for the 20 lowest eigenvalues and eigenvectors in 6380 CPU-seconds on an IBM-RISC 6000/340 workstation. We used a blocksize of $r = 8$, a range parameter of $\Delta = 5$, and a Chebyshev tolerance of $\delta = 0.1$. The results are shown in Table V.

The accuracy achieved is at least 11 figures for all calculated eigenvalues. The ability of the method to deal with highly degenerate eigenvalues is clearly demonstrated.

2. *Three Coupled Anharmonic Oscillators*

As a second three-dimensional example, we consider the potential for three coupled anharmonic sextic oscillators [17]

$$V(x, y, z) = V_6(x) + V_6(y) + V_6(z) + xy + xz + yz. \tag{41}$$

We have calculated the lowest 10 eigenstates and eigenvalues using a $32 \times 32 \times 32$ grid in $[-4, 4] \times [-4, 4] \times [-4, 4]$, a block size of $r = 2$, a range parameter of $\Delta = 20$, and a Chebyshev tolerance of $\delta = 0.1$. This calculation took 2700 CPU-seconds on an IBM-RISC 6000/340 worksta-

TABLE VI

The 10 Lowest Eigenvalues for a System of Three Coupled Sextic Anharmonic Oscillators (Kaluza only calculated states with positive parity and exchange quantum numbers.)

i	Kaluza [17]	present	difference
1	2.978302656836950	2.978302657465	$0.63\ 10^{-9}$
2		5.295992340812	
3		5.295992340812	
4		5.865822199388	
5		7.753739620670	
6		7.753739620670	
7	8.09166910	8.091658558754	$-0.11\ 10^{-4}$
8		8.871108060053	
9		8.871108060062	
10	9.114866	9.114771912692	$-0.94\ 10^{-4}$

tion. The results for the eigenvalues are shown in Table VI. It is seen that our ground state energy agrees with the result of Kaluza to nine figures.

IV. CONCLUSIONS

We presented a method that combines the advantages of the Chebyshev approximation for the $\exp(-H/\Delta)$ operator and the efficiency of the block–Lanczos method. Furthermore, the fast sine transform is employed which satisfies the bound state boundary conditions by construction. The resulting scheme is quite efficient in calculating low-lying eigenstates. Moreover, comparison of our results with analytic solutions of model problems and with results obtained via other competing methods, reveals that it is accurate as well.

ACKNOWLEDGMENTS

Two of us (D.G.P. and I.E.L.) gratefully acknowledge the financial support from Foundation for Research Development F.R.D. and University of South Africa (UNISA). We are also grateful to UNISA colleagues for their warm hospitality.

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