The confined system approximation for solving non-separable potentials in three dimensions

1998 J. Phys. A: Math. Gen. 31 3095

(http://iopscience.iop.org/0305-4470/31/13/013)

J. Phys. A: Math. Gen. **31** (1998) 3095–3114. Printed in the UK PII: S0305-4470(98)86382-8

The confined system approximation for solving non-separable potentials in three dimensions

H Taşeli and R Eid†

Department of Mathematics, Middle East Technical University, 06531 Ankara, Turkey

Received 29 July 1997, in final form 6 January 1998

Abstract. The Hilbert space $L_2(\mathbb{R}^3)$, to which the wavefunction of the three-dimensional Schrödinger equation belongs, has been replaced by $L_2(\Omega)$, where Ω is a bounded region. The energy spectrum of the usual unbounded system is then determined by showing that the Dirichlet and Neumann problems in $L_2(\Omega)$ generate upper and lower bounds, respectively, to the eigenvalues required. Highly accurate numerical results for the quartic and sextic oscillators are presented for a wide range of the coupling constants.

1. Introduction

The determination of the spectra of one-dimensional quantum oscillators is 30-year old science with many reliable methods developed to cope with the associated computational problem [1–6]. In spite of the existence of several moment-based asymptotic [3, 7] and perturbative [8–12] eigenenergy estimation techniques in two dimensions, however, the problem is still interesting from both numerical and theoretical viewpoints. In fact, a perturbation series expansion over the classical harmonic oscillator solution is divergent-asymptotic, which was verified explicitly by Bender and Wu [13] in their important investigation into the quartic oscillator. Therefore, the methods starting with the use of a harmonic-like reference function usually show weak convergence properties, especially for strong anharmonic couplings [10, 12].

On the other hand, studies on the three-dimensional perturbed oscillators are rather limited, and few reported results are available in the literature [14]. Because most of the methods lead to the evaluation of multiple-infinite series or recursions, the solution of the wave equation in higher-dimensional spaces is quite complicated. Fortunately, the difficulty has been lessened considerably by the advent of powerful computers.

In the preceding articles, Taşeli and co-workers [15–19] have focused on truncating the infinite domain of the Schrödinger equation and modifying asymptotic conditions at infinity. In one and two dimensions, it was shown that the Dirichlet and Neumann problems yield an excellent accuracy through converging upper and lower bounds to the energy levels of the corresponding unbounded system. Thus the present paper deals mainly with a straightforward generalization and extension of these earlier works to the more challenging three-dimensional eigenvalue problems.

We consider the appropriately scaled Schrödinger equation in the form

$$[-\nabla^2 + V(x, y, z)]\Psi(x, y, z) = E\Psi(x, y, z) \qquad \Psi \in L_2(\mathbb{R}^3) \tag{1.1}$$

† Present address: Department of Mathematics, Çankaya University, 06530 Ankara, Turkey.

with a general polynomial potential of degree M

$$V(x, y, z) = \sum_{m=1}^{M} v_{2m} \sum_{l=0}^{m} \binom{m}{l} \sum_{k=0}^{l} \binom{l}{k} a_{m-l,l-k,k} x^{2(m-l)} y^{2(l-k)} z^{2k} \qquad v_{2M} > 0 \tag{1.2}$$

in x^2, y^2 and z^2, where v_{2m} and $a_{m-l,l-k,k}$ are the coupling constants. The domain $\mathbb{R}^3$ is truncated to a bounded domain, which is defined as a cubic box of sides 2ℓ units length,

$$\Omega = \{(x, y, z) : -\ell \leqslant x, y, z \leqslant \ell\} \tag{1.3}$$

preserving the symmetry of the original unbounded domain about the origin. Therefore, the potential in (1.2) has clearly the reflection symmetries

$$V(x, y, z) = V(\pm x, \pm y, \pm z) \tag{1.4}$$

and, furthermore, interchange symmetries of three coordinates

$$V(x, y, z) = V(x, z, y) = V(y, x, z) = V(y, z, x) = V(z, x, y) = V(z, y, x) \tag{1.5}$$

provided that

$$a_{m-l,l-k,k} = a_{m-l,k,l-k} = a_{l-k,m-l,k} = a_{l-k,k,m-l} = a_{k,m-l,l-k} = a_{k,l-k,m-l} \tag{1.6}$$

for $m = 1, 2, \ldots, M$, $l = 0, 1, \ldots, m$, and $k = 0, 1, \ldots, l$. Note that the wavefunction $\Psi(x, y, z)$ will then satisfy the same symmetries as well.

As indicated, we assume the Dirichlet

$$\Psi(\pm\ell, y, z) = \Psi(x, \pm\ell, z) = \Psi(x, y, \pm\ell) = 0 \tag{1.7}$$

and Neumann conditions

$$\Psi_x(\pm\ell, y, z) = \Psi_y(x, \pm\ell, z) = \Psi_z(x, y, \pm\ell) = 0 \tag{1.8}$$

over the surfaces of the box. Now the eigenvalues of (1.1) in Ω may be regarded as a function of the confinement parameter ℓ. So if they are denoted by $E^+(\ell)$ in the case of the Dirichlet conditions, then it can be shown, in analogy with the one- and two-dimensional problems [17, 18], that

$$\begin{aligned}\frac{\mathrm{d}E^+}{\mathrm{d}\ell} = {}& -2\int_{-\ell}^{\ell}\int_{-\ell}^{\ell} \Psi_x^2(\ell, y, z)\,\mathrm{d}y\,\mathrm{d}z - 2\int_{-\ell}^{\ell}\int_{-\ell}^{\ell} \Psi_y^2(x, \ell, z)\,\mathrm{d}x\,\mathrm{d}z \\ & -2\int_{-\ell}^{\ell}\int_{-\ell}^{\ell} \Psi_z^2(x, y, \ell)\,\mathrm{d}x\,\mathrm{d}y\end{aligned} \tag{1.9}$$

and that $\mathrm{d}E^+/\mathrm{d}\ell$ is definitely negative (see the appendix). Thus the eigenenergies $E^+(\ell)$ of the Dirichlet problem decrease monotonically as ℓ increases providing upper bounds to those of the unbounded system, where $\ell \to \infty$.

In a similar fashion, the eigenvalues, $E^-(\ell)$ say, of the Neumann problem lead to the relation

$$\begin{aligned}\frac{\mathrm{d}E^-}{\mathrm{d}\ell} = {}& 2\int_{-\ell}^{\ell}\int_{-\ell}^{\ell} \{[V(\ell, y, z) - E^-]\Psi^2(\ell, y, z) + \Psi_y^2(\ell, y, z) + \Psi_z^2(\ell, y, z)\}\,\mathrm{d}y\,\mathrm{d}z \\ & +2\int_{-\ell}^{\ell}\int_{-\ell}^{\ell} \{[V(x, \ell, z) - E^-]\Psi^2(x, \ell, z) + \Psi_x^2(x, \ell, z) + \Psi_z^2(x, \ell, z)\}\,\mathrm{d}x\,\mathrm{d}z \\ & +2\int_{-\ell}^{\ell}\int_{-\ell}^{\ell} \{[V(x, y, \ell) - E^-]\Psi^2(x, y, \ell) + \Psi_x^2(x, y, \ell) + \Psi_y^2(x, y, \ell)\}\,\mathrm{d}x\,\mathrm{d}y\end{aligned} \tag{1.10}$$

which remains strictly positive, if $|\ell|$ is beyond the classical turning points (see the appendix). It should be noted that this restriction on the confinement parameter ℓ is not necessary but sufficient to make $\mathrm{d}E^-/\mathrm{d}\ell$ always positive. Therefore, the eigenvalues of the Neumann problem is an increasing function of ℓ yielding lower bounds to the asymptotic eigenvalues.

In the appendix, an explicit proof on the decreasing and increasing behaviour of $E(\ell)$ stated by (1.9) and (1.10) is presented. As an important consequence, the Dirichlet and Neumann boundary value problems generate error bounds to the energy levels of the usual system on $\mathbb{R}^3$, in the sense that

$$E^-(\ell) < E < E^+(\ell). \tag{1.11}$$

Hence, in section 2 we establish a variational method by means of simple trigonometric basis functions to determine E^+ as well as E^- for an arbitrary polynomial in (1.2). In section 3, the procedure is applied to particular problems including the quartic and sextic oscillators. The last section concludes the paper with a discussion of the results.

2. Variational formulation with simple trigonometric bases

By introducing the coordinate transformations,

$$\xi = \frac{\pi}{\ell}x \qquad \eta = \frac{\pi}{\ell}y \qquad \zeta = \frac{\pi}{\ell}z \tag{2.1}$$

the Schrödinger equation in (1.1) becomes

$$[-\nabla^2 + \nu^2 V(\nu\xi, \nu\eta, \nu\zeta)]\Psi(\xi, \eta, \zeta) = \nu^2 E(\ell)\Psi(\xi, \eta, \zeta) \qquad \nu = \frac{\ell}{\pi} \tag{2.2}$$

with the scaled domain Ω,

$$\Omega = \{(\xi, \eta, \zeta) : -\pi \leqslant \xi, \eta, \zeta \leqslant \pi\}. \tag{2.3}$$

If we first consider the wave equation for the motion of a free particle

$$\frac{\partial^2\Psi}{\partial\xi^2} + \frac{\partial^2\Psi}{\partial\eta^2} + \frac{\partial^2\Psi}{\partial\zeta^2} + \lambda\Psi(\xi, \eta, \zeta) = 0 \tag{2.4}$$

where the potential has been taken as

$$V(\xi, \eta, \zeta) = \begin{cases} 0 & \text{inside } \Omega \\ \infty & \text{outside } \Omega \end{cases} \tag{2.5}$$

it is an easy matter to obtain exact analytical eigensolutions. Thus the normalized sequences of functions

$$\phi_{ijk}(\xi, \eta, \zeta) = \pi^{-3/2}\cos(i + \tfrac{1}{2})\xi\ \cos(j + \tfrac{1}{2})\eta\ \cos(k + \tfrac{1}{2})\zeta \tag{2.6a}$$
$$\phi_{ijk}(\xi, \eta, \zeta) = \pi^{-3/2}\cos(i + \tfrac{1}{2})\xi\ \cos(j + \tfrac{1}{2})\eta\ \sin(k + 1)\zeta \tag{2.6b}$$
$$\phi_{ijk}(\xi, \eta, \zeta) = \pi^{-3/2}\cos(i + \tfrac{1}{2})\xi\ \sin(j + 1)\eta\ \cos(k + \tfrac{1}{2})\zeta \tag{2.6c}$$
$$\phi_{ijk}(\xi, \eta, \zeta) = \pi^{-3/2}\sin(i + 1)\xi\ \cos(j + \tfrac{1}{2})\eta\ \cos(k + \tfrac{1}{2})\zeta \tag{2.6d}$$
$$\phi_{ijk}(\xi, \eta, \zeta) = \pi^{-3/2}\sin(i + 1)\xi\ \sin(j + 1)\eta\ \cos(k + \tfrac{1}{2})\zeta \tag{2.6e}$$
$$\phi_{ijk}(\xi, \eta, \zeta) = \pi^{-3/2}\sin(i + 1)\xi\ \cos(j + \tfrac{1}{2})\eta\ \sin(k + 1)\zeta \tag{2.6f}$$
$$\phi_{ijk}(\xi, \eta, \zeta) = \pi^{-3/2}\cos(i + \tfrac{1}{2})\xi\ \sin(j + 1)\eta\ \sin(k + 1)\zeta \tag{2.6g}$$

and

$$\phi_{ijk}(\xi,\eta,\zeta) = \pi^{-3/2}\sin(i+1)\xi\ \sin(j+1)\eta\ \sin(k+1)\zeta \tag{2.6h}$$

satisfy (2.4) and the Dirichlet boundary conditions when λ values are properly chosen for all $i, j, k = 0, 1, \ldots$. Furthermore, the functions

$$\varphi_{ijk}(\xi,\eta,\zeta) = \mathcal{N}_{ijk}\,\pi^{-3/2}\ \cos i\xi\ \cos j\eta\ \cos k\zeta \tag{2.7a}$$

$$\varphi_{ijk}(\xi,\eta,\zeta) = \sqrt{2}\,\mathcal{N}_{i,j,0}\,\pi^{-3/2}\ \cos i\xi\ \cos j\eta\ \sin(k+\tfrac{1}{2})\zeta \tag{2.7b}$$

$$\varphi_{ijk}(\xi,\eta,\zeta) = \sqrt{2}\,\mathcal{N}_{i,0,k}\,\pi^{-3/2}\ \cos i\xi\ \sin(j+\tfrac{1}{2})\eta\ \cos k\zeta \tag{2.7c}$$

$$\varphi_{ijk}(\xi,\eta,\zeta) = \sqrt{2}\,\mathcal{N}_{0,j,k}\,\pi^{-3/2}\ \sin(i+\tfrac{1}{2})\xi\ \cos j\eta\ \cos k\zeta \tag{2.7d}$$

$$\varphi_{ijk}(\xi,\eta,\zeta) = 2\,\mathcal{N}_{0,0,k}\,\pi^{-3/2}\ \sin(i+\tfrac{1}{2})\xi\ \sin(j+\tfrac{1}{2})\eta\ \cos k\zeta \tag{2.7e}$$

$$\varphi_{ijk}(\xi,\eta,\zeta) = 2\,\mathcal{N}_{0,j,0}\,\pi^{-3/2}\ \sin(i+\tfrac{1}{2})\xi\ \cos j\eta\ \sin(k+\tfrac{1}{2})\zeta \tag{2.7f}$$

$$\varphi_{ijk}(\xi,\eta,\zeta) = 2\,\mathcal{N}_{i,0,0}\,\pi^{-3/2}\ \cos i\xi\ \sin(j+\tfrac{1}{2})\eta\ \sin(k+\tfrac{1}{2})\zeta \tag{2.7g}$$

and

$$\varphi_{ijk}(\xi,\eta,\zeta) = \pi^{-3/2}\ \sin(i+\tfrac{1}{2})\xi\ \sin(j+\tfrac{1}{2})\eta\ \sin(k+\tfrac{1}{2})\zeta \tag{2.7h}$$

are solutions of (2.4) with Neumann conditions, where $\mathcal{N}_{ijk}$ is a normalization constant defined by

$$\mathcal{N}_{ijk} = [(1+\delta_{i,0})(1+\delta_{j,0})(1+\delta_{k,0})]^{-1/2} \tag{2.8}$$

in which δ_{ij} stands for the Kronecker delta. The 16 sets of functions in (2.6) and (2.7) comprise complete orthonormal bases for the Hilbert space $L_2(\Omega)$ which, henceforth, are referred to as $\mathbb{S}_1^+$, $\mathbb{S}_2^+$, $\mathbb{S}_3^+$, $\mathbb{S}_4^+$, $\mathbb{S}_5^+$, $\mathbb{S}_6^+$, $\mathbb{S}_7^+$, $\mathbb{S}_8^+$ and $\mathbb{S}_1^-$, $\mathbb{S}_2^-$, $\mathbb{S}_3^-$, $\mathbb{S}_4^-$, $\mathbb{S}_5^-$, $\mathbb{S}_6^-$, $\mathbb{S}_7^-$, $\mathbb{S}_8^-$, respectively.

On the other hand, since the wavefunction of the full Schrödinger equation (2.2) belongs to the same space spanned by the ϕ_{ijk} or φ_{ijk}, we can propose the solutions

$$\Phi^+(\xi,\eta,\zeta) = \sum_{i=0}^{\infty}\sum_{j=0}^{\infty}\sum_{k=0}^{\infty} h_{ijk}\ \phi_{ijk}(\xi,\eta,\zeta) \tag{2.9}$$

and

$$\Phi^-(\xi,\eta,\zeta) = \sum_{i=0}^{\infty}\sum_{j=0}^{\infty}\sum_{k=0}^{\infty} f_{ijk}\ \varphi_{ijk}(\xi,\eta,\zeta) \tag{2.10}$$

for the Dirichlet and Neumann problems, respectively, where h_{ijk} and f_{ijk} are the expansion coefficients. The energy levels of a three-dimensional oscillator being considered are characterized by three quantum numbers n_1, n_2 and n_3, i.e. $E \equiv E_{n_1n_2n_3}$. The spectrum can be decomposed into eight subsets owing to the reflection symmetries of the potential in (1.2). It is worth mentioning that the structures of the present bases give the possibility of taking care of these subsets individually in a natural way. In fact, the sets $\mathbb{S}_1^+$ ($\mathbb{S}_1^-$) and $\mathbb{S}_8^+$ ($\mathbb{S}_8^-$) can be used in the expansions (2.9) or (2.10) to determine the discrete states with the same parity, namely, three even or three odd. However, the eigenvalues with mixed parity, two even and one odd or one even and two odd, should be investigated by means of the others.

Hence the substitution of (2.9) into (2.2) reduces the Schrödinger equation to the secular equations

$$\sum_{l=0}^{\infty}\sum_{m=0}^{\infty}\sum_{n=0}^{\infty}[H_{ijklmn} - \nu^2 E^+(\ell)\delta_{il}\delta_{jm}\delta_{kn}]h_{lmn} = 0 \tag{2.11}$$

for $i, j, k = 0, 1, \ldots,$ with

$$H_{ijklmn} = \int_{-\pi}^{\pi}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi} \phi_{lmn}[-\nabla^2 + \nu^2 V(\nu\xi, \nu\eta, \nu\zeta)]\phi_{ijk}\, \mathrm{d}\xi\, \mathrm{d}\eta\, \mathrm{d}\zeta. \tag{2.12}$$

The entries H_{ijklmn} are nicely written in a compact form

$$\begin{aligned} H_{ijklmn} = {}& \frac{1}{4}\left[(2i+1+p_1)^2 + (2j+1+p_2)^2 + (2k+1+p_3)^2\right]\delta_{il}\delta_{jm}\delta_{kn} \\ & + \nu^2 \sum_{I=1}^{M} v_{2I}\nu^{2I} \sum_{J=0}^{I}\binom{I}{J}\sum_{K=0}^{J}\binom{J}{K} a_{I-J,J-K,K}[R_{i-l}^{(I-J)} + s_1 R_{i+l+1+p_1}^{(I-J)}] \\ & \times[R_{j-m}^{(J-K)} + s_2 R_{j+m+1+p_2}^{(J-K)}][R_{k-n}^{(K)} + s_3 R_{k+n+1+p_3}^{(K)}] \end{aligned} \tag{2.13}$$

where $R_k^{(j)}$ denote the simple integrals of the type

$$R_k^{(j)} = \frac{1}{\pi}\int_0^{\pi} \theta^{2j}\cos k\theta\, \mathrm{d}\theta. \tag{2.14}$$

In this definition of H_{ijklmn} we have introduced the integer parameters s_1, s_2, s_3, p_1, p_2 and p_3 to include every basis in (2.6), such that

$$s_1 = s_2 = s_3 = 1 \qquad p_1 = p_2 = p_3 = 0 \tag{2.15a}$$

$$s_1 = s_2 = 1 \quad s_3 = -1 \qquad p_1 = p_2 = 0 \quad p_3 = 1 \tag{2.15b}$$

$$s_1 = 1 \quad s_2 = -1 \quad s_3 = 1 \qquad p_1 = 0 \quad p_2 = 1 \quad p_3 = 0 \tag{2.15c}$$

$$s_1 = 1 \quad s_2 = s_3 = -1 \qquad p_1 = 0 \quad p_2 = p_3 = 1 \tag{2.15d}$$

$$s_1 = -1 \quad s_2 = s_3 = 1 \qquad p_1 = 1 \quad p_2 = p_3 = 0 \tag{2.15e}$$

$$s_1 = 1 \quad s_2 = 1 \quad s_3 = -1 \qquad p_1 = 1 \quad p_2 = 0 \quad p_3 = 1 \tag{2.15f}$$

$$s_1 = s_2 = -1 \quad s_3 = 1 \qquad p_1 = p_2 = 1 \quad p_3 = 0 \tag{2.15g}$$

and

$$s_1 = s_2 = s_3 = -1 \qquad p_1 = p_2 = p_3 = 1 \tag{2.15h}$$

for the sets, $\mathbb{S}_1^+$–$\mathbb{S}_7^+$ and $\mathbb{S}_8^+$, respectively.

Starting from the solution $\Phi^-(\xi, \eta, \zeta)$, which obeys the Neumann conditions, we obtain again an algebraic system of equations in the form

$$\sum_{l=0}^{\infty}\sum_{m=0}^{\infty}\sum_{n=0}^{\infty}[F_{ijklmn} - \nu^2 E^-(\ell)\delta_{il}\delta_{jm}\delta_{kn}]f_{lmn} = 0 \tag{2.16}$$

for $i, j, k = 0, 1, \ldots,$ with

$$\begin{aligned} F_{ijklmn} = {}& \frac{1}{4}[(2i+p_1)^2 + (2j+p_2)^2 + (2k+p_3)^2]\delta_{il}\delta_{jm}\delta_{kn} \\ & + \sigma\nu^2 \sum_{I=1}^{M} v_{2I}\nu^{2I} \sum_{J=0}^{I}\binom{I}{J}\sum_{K=0}^{J}\binom{J}{K} a_{I-J,J-K,K}[R_{i-l}^{(I-J)} + s_1 R_{i+l+p_1}^{(I-J)}] \\ & \times[R_{j-m}^{(J-K)} + s_2 R_{j+m+p_2}^{(J-K)}][R_{k-n}^{(K)} + s_3 R_{k+n+p_3}^{(K)}]. \end{aligned} \tag{2.17}$$

Here, the parameters s_1, s_2, s_3, p_1, p_2 and p_3 defined by (2.15) are also used for the Neumann basis sets in (2.7). Moreover, an additional adjustable parameter σ has been introduced which should be taken as

$$\sigma = \mathcal{N}_{ijk}\mathcal{N}_{lmn} \qquad \sigma = 2\mathcal{N}_{i,j,0}\mathcal{N}_{l,m,0} \qquad \sigma = 2\mathcal{N}_{i,0,k}\mathcal{N}_{l,0,n} \qquad \sigma = 2\mathcal{N}_{0,j,k}\mathcal{N}_{0,m,n} \tag{2.18a}$$

and

$$\sigma = 4\mathcal{N}_{i,0,0}\mathcal{N}_{l,0,0} \qquad \sigma = 4\mathcal{N}_{0,j,0}\mathcal{N}_{0,m,0} \qquad \sigma = 4\mathcal{N}_{0,0,k}\mathcal{N}_{0,0,n} \qquad \sigma = 1 \tag{2.18b}$$

for $\mathbb{S}_1^-$–$\mathbb{S}_4^-$ and $\mathbb{S}_5^-$–$\mathbb{S}_8^-$, respectively.

On the numerical side of the work, we deal with the truncated solutions

$$\Phi^+(\xi, \eta, \zeta) = \sum_{i=0}^{N-1}\sum_{j=0}^{N-1}\sum_{k=0}^{N-1} h_{ijk}\,\phi_{ijk}(\xi, \eta, \zeta) \tag{2.19}$$

and

$$\Phi^-(\xi, \eta, \zeta) = \sum_{i=0}^{N-1}\sum_{j=0}^{N-1}\sum_{k=0}^{N-1} f_{ijk}\,\varphi_{ijk}(\xi, \eta, \zeta) \tag{2.20}$$

where N is the truncation order. In this case, the equations in (2.11) and (2.16) describe finite algebraic systems of order N^3. As long as N remains finite it can be deduced, by recoding the indexes of H_{ijklmn} and F_{ijklmn}, that these systems are expressible in the form of standard matrix eigenvalue problems. In fact, if we define the integer transformation T, $T : \mathbb{N}_0^6 \to \mathbb{N}^2$,

$$\begin{aligned} T = \{(I, J) \in \mathbb{N}^2 : I = lN^2 + mN + n + 1 \text{ and } J = iN^2 + jN + k + 1,\\ \forall(i, j, k, l, m, n) \in \mathbb{N}_0^6\} \end{aligned} \tag{2.21}$$

then H_{ijklmn} (F_{ijklmn}) and $\delta_{il}\delta_{jm}\delta_{kn}$ are converted to a matrix $[\mathcal{A}_{IJ}]$ and the identity matrix $[\delta_{IJ}]$ of orders N^3, respectively, where $\mathbb{N} = \{1, 2, \ldots\}$ is a subset of the set of natural numbers and $\mathbb{N}_0 = \{0\} \cup \mathbb{N}$. Similarly, the mapping S, $S : \mathbb{N}_0^3 \to \mathbb{N}$,

$$S = \{J \in \mathbb{N} : J = iN^2 + jN + k + 1, \quad \forall\,(i, j, k) \in \mathbb{N}_0^3\} \tag{2.22}$$

transforms h_{ijk} (f_{ijk}) with $i, j, k = 0, 1, \ldots, N-1$ into b_J with $J = 1, 2, \ldots, N^3$. Hence we may represent (2.11) and (2.16) in the form

$$\sum_{J=1}^{N^3}(\mathcal{A}_{IJ} - \nu^2 E\,\delta_{IJ})b_J = 0 \qquad I = 1, 2, \ldots, N^3. \tag{2.23}$$

It should be noted that the matrix $[\mathcal{A}_{IJ}]$ is symmetric due to the block symmetry of H_{ijklmn} (F_{ijklmn}), i.e. $H_{ijklmn} = H_{lmnijk}$ ($F_{ijklmn} = F_{lmnijk}$).

3. Applications to quartic and sextic oscillators

The generalized anharmonic oscillators are being investigated with considerable intensity, motivated by quantum mechanical problems in field theory and molecular physics. A detailed review of the anharmonic eigenvalue problems is outside the scope of this article, but they provide a convenient testing ground for the present approximation.

In table 1, we calculate the ground-state eigenvalue of the quartic oscillator,

$$V(x, y, z) = x^2y^2 + x^2z^2 + y^2z^2 \tag{3.1}$$

to illustrate how the method can be applied in finding error bounds as the confinement parameter ℓ varies. To denote lower and upper bound results we employ the notation wherein, for example, 1/3 means that the eigenvalue is bounded by $1 < E_{0,0,0} < 3$, if $\ell = 2.0$. Similarly, 2.169 856 706 36/95 at $\ell = 6.05$ implies more rigorous two-sided bounds such that $2.169\,856\,706\,36 < E_{0,0,0} < 2.169\,856\,706\,95$. As another specific example, we examine the lowest three energy levels of the sextic oscillator

$$V(x, y, z) = x^2 + y^2 + z^2 + v_6(x^6 + y^6 + z^6 + 6x^2y^2z^2) \tag{3.2}$$

Table 1. Lower and upper bounds to the ground-state eigenvalue of the quartic oscillator in (3.1), as a function of the confinement parameter ℓ.

ℓ	N	$E_{0,0,0}$
2.00	4	1/3
2.50	4	2.105/228
3.00	5	2.1598/788
3.50	6	2.1686/710
4.00	7	2.169 74/97
4.50	9	2.169 847/66
5.00	11	2.169 8561/74
5.50	12	2.169 856 68/73
5.75	13	2.169 856 700/14
6.05	14	2.169 856 706 36/95

Table 2. Lower and upper bounds to the first three eigenvalues of the sextic oscillator in (3.2) where $v_6 = 10^6$, as a function of the confinement parameter ℓ.

ℓ	N	$E_{0,0,0}$	$E_{0,0,1} = E_{0,1,0} = E_{1,0,0}$	$E_{1,1,0} = E_{1,0,1} = E_{0,1,1}$
0.325	5	112/4	218/22	330/6
0.350	5	113.24/43	219/21	333/5
0.375	6	113.333/51	220.025/74	333.665/773
0.400	7	113.3423/33	220.0497/524	333.6998/7035
0.425	9	113.342 760/87	220.051 079/161	333.701 666/778
0.450	11	113.342 773 57/97	220.051 120 77/202	333.701 723 21/491
0.475	12	113.342 773 7740/72	220.051 121 407/17	333.701 724 080/94
0.485	13	113.342 773 775 18/23	220.051 121 4116/23	333.701 724 0866/76

in the same manner to check if there is any difficulty in passing from a quartic oscillator to such a sextic oscillator with a very large v_6 value of 10^6 (table 2).

For the sake of a systematic numerical analysis, we may consider the general form of a quartic oscillator which is obtainable from (1.2) with $M = 2$. If we assume the interchange symmetries in (1.5) of the coordinates and introduce a simple scaling transformation, this potential can be written concisely in the form

$$V(x, y, z) = x^2 + y^2 + z^2 + c_4[x^4 + y^4 + z^4 + 2\alpha(x^2y^2 + x^2z^2 + y^2z^2)] \tag{3.3}$$

involving only two effective coupling constants c_4 and α. It is apparent that for a non-negative quartic anharmonicity c_4 should be necessarily positive. The case of $c_4 = 0$ leads to the harmonic oscillator which is trivial. Moreover, the condition

$$\alpha \geqslant -\tfrac{1}{2} \tag{3.4}$$

is sufficient to make the potential bounded below. In the two-dimensional problems, it is possible to find unitary transformations which suggest that the eigenvalue equation can be investigated in the range of α, $-1 \leqslant \alpha \leqslant 1$, without any loss of generality [9, 18]. Unfortunately, however, there are no such transformations in three-dimensional space, and the only restriction on α is given by (3.4). Therefore, the lower and upper bound energy levels of the quartic oscillator are reported for c_4 values of 10^{-3}, 1, and 10^3 in tables 3, 4 and 5, respectively, as a function of α by taking $\alpha = -\frac{1}{2}, 0, 1$ and 10.

Finally, we deal with the sextic oscillator in (1.2), where $v_4 = 0$ and $M = 3$. On making use of a linear scaling and taking advantage of the interchange symmetries of the

Table 3. Lower and upper bounds to the eigenvalues of the quartic oscillator in (3.3), where $c_4 = 10^{-3}$, as a function of α.

α	ℓ_{cr}	N	$\{n_1, n_2, n_3\}$	$E_{n_1 n_2 n_3}$	Basis set
$-\frac{1}{2}$	5.50	11	{0, 0, 0}	3.001 497 851 40/1	$\mathbb{S}_1^-/\mathbb{S}_1^+$
	5.80	11	{0, 0, 1} – {0, 1, 0} – {1, 0, 0}	5.003 492 259 84/5	$\mathbb{S}_2^-/\mathbb{S}_2^+ - \mathbb{S}_3^-/\mathbb{S}_3^+ - \mathbb{S}_4^-/\mathbb{S}_4^+$
	5.70	11	{1, 1, 0} – {1, 0, 1} – {0, 1, 1}	7.004 490 764 08/10	$\mathbb{S}_5^-/\mathbb{S}_5^+ - \mathbb{S}_6^-/\mathbb{S}_6^+ - \mathbb{S}_7^-/\mathbb{S}_7^+$
	5.86	11	{0, 0, 2}	7.007 471 819 65/7	$\mathbb{S}_1^-/\mathbb{S}_1^+$
	5.87	11	{0, 2, 0} – {2, 0, 0}	7.008 969 294 02/3	$\mathbb{S}_1^-/\mathbb{S}_1^+ - \mathbb{S}_1^-/\mathbb{S}_1^+$
	5.70	11	{1, 1, 1}	9.004 491 880 91/5	$\mathbb{S}_8^-/\mathbb{S}_8^+$
	6.05	12	{0, 2, 1} – {0, 1, 2} – {1, 0, 2}	9.007 802 185 74/6	$\mathbb{S}_2^-/\mathbb{S}_2^+ - \mathbb{S}_3^-/\mathbb{S}_3^+ - \mathbb{S}_4^-/\mathbb{S}_4^+$
	6.05	12	{2, 0, 1} – {2, 1, 0} – {1, 2, 0}	9.008 974 855 87/9	$\mathbb{S}_2^-/\mathbb{S}_2^+ - \mathbb{S}_3^-/\mathbb{S}_3^+ - \mathbb{S}_4^-/\mathbb{S}_4^+$
	6.05	12	{0, 0, 3} – {0, 3, 0} – {3, 0, 0}	9.016 592 212 86/99	$\mathbb{S}_2^-/\mathbb{S}_2^+ - \mathbb{S}_3^-/\mathbb{S}_3^+ - \mathbb{S}_4^-/\mathbb{S}_4^+$
0	5.50	11	{0, 0, 0}	3.002 246 078 01/3	$\mathbb{S}_1^-/\mathbb{S}_1^+$
	5.70	11	{0, 0, 1} – {0, 1, 0} – {1, 0, 0}	5.005 237 133 51/2	$\mathbb{S}_2^-/\mathbb{S}_2^+ - \mathbb{S}_3^-/\mathbb{S}_3^+ - \mathbb{S}_4^-/\mathbb{S}_4^+$
	5.80	11	{1, 1, 0} – {1, 0, 1} – {0, 1, 1}	7.008 228 189 00/2	$\mathbb{S}_5^-/\mathbb{S}_5^+ - \mathbb{S}_6^-/\mathbb{S}_6^+ - \mathbb{S}_7^-/\mathbb{S}_7^+$
	5.90	12	{0, 0, 2} – {0, 2, 0} – {2, 0, 0}	7.011 209 258 11/6	$\mathbb{S}_1^-/\mathbb{S}_1^+ - \mathbb{S}_1^-/\mathbb{S}_1^+ - \mathbb{S}_1^-/\mathbb{S}_1^+$
	5.70	11	{1, 1, 1}	9.011 219 244 49/53	$\mathbb{S}_8^-/\mathbb{S}_8^+$
	6.05	12	{0, 2, 1} – {0, 1, 2} – {1, 0, 2} –	9.014 200 313 62/4	$\mathbb{S}_2^-/\mathbb{S}_2^+ - \mathbb{S}_3^-/\mathbb{S}_3^+ - \mathbb{S}_4^-/\mathbb{S}_4^+ -$
			{2, 0, 1} – {2, 1, 0} – {1, 2, 0}		$\mathbb{S}_2^-/\mathbb{S}_2^+ - \mathbb{S}_3^-/\mathbb{S}_3^+ - \mathbb{S}_4^-/\mathbb{S}_4^+$
	6.05	12	{0, 0, 3} – {0, 3, 0} – {3, 0, 0}	9.020 149 977 33/47	$\mathbb{S}_2^-/\mathbb{S}_2^+ - \mathbb{S}_3^-/\mathbb{S}_3^+ - \mathbb{S}_4^-/\mathbb{S}_4^+$
1	5.50	11	{0, 0, 0}	3.003 739 748 16/8	$\mathbb{S}_1^-/\mathbb{S}_1^+$
	5.80	11	{0, 0, 1} – {0, 1, 0} – {1, 0, 0}	5.008 717 444 47/8	$\mathbb{S}_2^-/\mathbb{S}_2^+ - \mathbb{S}_3^-/\mathbb{S}_3^+ - \mathbb{S}_4^-/\mathbb{S}_4^+$
	5.80	11	{1, 1, 0} – {1, 0, 1} – {0, 1, 1} –	7.015 675 918 90/1	$\mathbb{S}_5^-/\mathbb{S}_5^+ - \mathbb{S}_6^-/\mathbb{S}_6^+ - \mathbb{S}_7^-/\mathbb{S}_7^+ -$
			{0, 0, 2} – {0, 2, 0}		$\mathbb{S}_1^-/\mathbb{S}_1^+ - \mathbb{S}_1^-/\mathbb{S}_1^+$
	5.80	11	{2, 0, 0}	7.018 652 592 02/10	$\mathbb{S}_1^-/\mathbb{S}_1^+$
	5.70	11	{0, 2, 1} – {0, 1, 2} – {1, 0, 2} –		$\mathbb{S}_2^-/\mathbb{S}_2^+ - \mathbb{S}_3^-/\mathbb{S}_3^+ - \mathbb{S}_4^-/\mathbb{S}_4^+ -$
			{1, 1, 1} –	9.024 609 354 58/62	$\mathbb{S}_8^-/\mathbb{S}_8^+ -$
			{2, 0, 1} – {2, 1, 0} – {1, 2, 0}		$\mathbb{S}_2^-/\mathbb{S}_2^+ - \mathbb{S}_3^-/\mathbb{S}_3^+ - \mathbb{S}_4^-/\mathbb{S}_4^+$
	5.90	11	{0, 0, 3} – {0, 3, 0} – {3, 0, 0}	9.029 559 527 40/70	$\mathbb{S}_2^-/\mathbb{S}_2^+ - \mathbb{S}_3^-/\mathbb{S}_3^+ - \mathbb{S}_4^-/\mathbb{S}_4^+$
	5.90	11	{1, 1, 2} – {1, 2, 1} – {2, 1, 1} –		$\mathbb{S}_5^-/\mathbb{S}_5^+ - \mathbb{S}_6^-/\mathbb{S}_6^+ - \mathbb{S}_7^-/\mathbb{S}_7^+ -$
			{0, 2, 2} – {2, 0, 2} – {2, 2, 0} –	11.035 511 979 7/801	$\mathbb{S}_1^-/\mathbb{S}_1^+ - \mathbb{S}_1^-/\mathbb{S}_1^+ - \mathbb{S}_1^-/\mathbb{S}_1^+ -$
			{1, 3, 0} – {1, 0, 3} – {0, 1, 3}		$\mathbb{S}_5^-/\mathbb{S}_5^+ - \mathbb{S}_6^-/\mathbb{S}_6^+ - \mathbb{S}_7^-/\mathbb{S}_7^+$
10	5.50	11	{0, 0, 0}	3.017 020 559 64/6	$\mathbb{S}_1^-/\mathbb{S}_1^+$
	5.80	11	{0, 0, 1} – {0, 1, 0} – {1, 0, 0}	5.039 496 417 84/5	$\mathbb{S}_2^-/\mathbb{S}_2^+ - \mathbb{S}_3^-/\mathbb{S}_3^+ - \mathbb{S}_4^-/\mathbb{S}_4^+$
	6.00	12	{0, 0, 2} – {0, 2, 0}	7.055 114 700 35/7	$\mathbb{S}_1^-/\mathbb{S}_1^+ - \mathbb{S}_1^-/\mathbb{S}_1^+$
	5.70	11	{1, 1, 0} – {1, 0, 1} – {0, 1, 1}	7.081 161 427 04/6	$\mathbb{S}_5^-/\mathbb{S}_5^+ - \mathbb{S}_6^-/\mathbb{S}_6^+ - \mathbb{S}_7^-/\mathbb{S}_7^+$
	6.00	12	{2, 0, 0}	7.083 853 177 49/51	$\mathbb{S}_1^-/\mathbb{S}_1^+$
	6.00	12	{0, 2, 1} – {0, 1, 2} – {1, 0, 2}	9.082 310 599 92/7	$\mathbb{S}_2^-/\mathbb{S}_2^+ - \mathbb{S}_3^-/\mathbb{S}_3^+ - \mathbb{S}_4^-/\mathbb{S}_4^+$
	6.00	12	{2, 0, 1} – {2, 1, 0} – {1, 2, 0}	9.115 917 452 33/5	$\mathbb{S}_2^-/\mathbb{S}_2^+ - \mathbb{S}_3^-/\mathbb{S}_3^+ - \mathbb{S}_4^-/\mathbb{S}_4^+$
	5.60	11	{1, 1, 1}	9.141 495 012 62/7	$\mathbb{S}_8^-/\mathbb{S}_8^+$
	6.10	12	{0, 0, 3} – {0, 3, 0} – {3, 0, 0}	9.144 988 944 00/2	$\mathbb{S}_2^-/\mathbb{S}_2^+ - \mathbb{S}_3^-/\mathbb{S}_3^+ - \mathbb{S}_4^-/\mathbb{S}_4^+$

coordinates, we again minimize the number of coupling constants. So the potential is characterized by the function

$$V(x, y, z) = x^2 + y^2 + z^2 + c_6[x^6 + y^6 + z^6 + 3\beta(x^4y^2 + x^4z^2 + x^2y^4 + x^2z^4 + y^4z^2 + y^2z^4) + 6\gamma x^2y^2z^2] \tag{3.5}$$

with three parameters c_6, β and γ. Here, $c_6 > 0$, and it can be shown after some algebra that

$$6\beta + 2\gamma \geqslant -1 \tag{3.6}$$

for a required non-negative sextic anharmonicity, if $\gamma \neq 1$. For $\gamma = 1$, we must have

$$\beta \geqslant -\tfrac{1}{3}. \tag{3.7}$$

Table 4. Lower and upper bounds to the eigenvalues of the quartic oscillator in (3.3), where $c_4 = 1$, as a function of α.

α	$\ell_{\rm cr}$	N	$\{n_1,\ n_2,\ n_3\}$	$E_{n_1 n_2 n_3}$	Basis set
$-\frac{1}{2}$	3.50	11	{0, 0, 0}	3.854 803 298 31/3	$\mathbb{S}_1^-/\mathbb{S}_1^+$
	3.65	12	{0, 0, 1} – {0, 1, 0} – {1, 0, 0}	6.730 816 582 27/8	$\mathbb{S}_2^-/\mathbb{S}_2^+ - \mathbb{S}_3^-/\mathbb{S}_3^+ - \mathbb{S}_4^-/\mathbb{S}_4^+$
	3.75	12	{1, 1, 0} – {1, 0, 1} – {0, 1, 1}	9.272 020 739 68/70	$\mathbb{S}_5^-/\mathbb{S}_5^+ - \mathbb{S}_6^-/\mathbb{S}_6^+ - \mathbb{S}_7^-/\mathbb{S}_7^+$
	3.65	12	{0, 0, 2}	9.949 866 733 32/49	$\mathbb{S}_1^-/\mathbb{S}_1^+$
	3.50	11	{0, 2, 0} – {2, 0, 0}	10.690 701 5341/5	$\mathbb{S}_1^-/\mathbb{S}_1^+ - \mathbb{S}_1^-/\mathbb{S}_1^+$
	3.65	11	{1, 1, 1}	11.412 029 2020/9	$\mathbb{S}_8^-/\mathbb{S}_8^+$
	3.65	12	{0, 2, 1} – {0, 1, 2} – {1, 0, 2}	12.305 529 1690/711	$\mathbb{S}_2^-/\mathbb{S}_2^+ - \mathbb{S}_3^-/\mathbb{S}_3^+ - \mathbb{S}_4^-/\mathbb{S}_4^+$
	3.65	12	{2, 0, 1} – {2, 1, 0} – {1, 2, 0}	13.076 148 8000/2	$\mathbb{S}_2^-/\mathbb{S}_2^+ - \mathbb{S}_3^-/\mathbb{S}_3^+ - \mathbb{S}_4^-/\mathbb{S}_4^+$
	3.75	12	{1, 1, 2} – {1, 2, 1} – {2, 1, 1}	14.378 446 5269/89	$\mathbb{S}_5^-/\mathbb{S}_5^+ - \mathbb{S}_6^-/\mathbb{S}_6^+ - \mathbb{S}_7^-/\mathbb{S}_7^+$
	3.65	12	{0, 0, 3} – {0, 3, 0} – {3, 0, 0}	14.779 954 4411/8	$\mathbb{S}_2^-/\mathbb{S}_2^+ - \mathbb{S}_3^-/\mathbb{S}_3^+ - \mathbb{S}_4^-/\mathbb{S}_4^+$
0	3.45	11	{0, 0, 0}	4.177 054 924 59/60	$\mathbb{S}_1^-/\mathbb{S}_1^+$
	3.45	11	{0, 0, 1} – {0, 1, 0} – {1, 0, 0}	7.433 515 987 26/9	$\mathbb{S}_2^-/\mathbb{S}_2^+ - \mathbb{S}_3^-/\mathbb{S}_3^+ - \mathbb{S}_4^-/\mathbb{S}_4^+$
	3.45	11	{1, 1, 0} – {1, 0, 1} – {0, 1, 1}	10.689 977 0499/500	$\mathbb{S}_5^-/\mathbb{S}_5^+ - \mathbb{S}_6^-/\mathbb{S}_6^+ - \mathbb{S}_7^-/\mathbb{S}_7^+$
	3.45	11	{0, 0, 2} – {0, 2, 0} – {2, 0, 0}	11.439 753 2407/10	$\mathbb{S}_1^-/\mathbb{S}_1^+ - \mathbb{S}_1^-/\mathbb{S}_1^+ - \mathbb{S}_1^-/\mathbb{S}_1^+$
	3.45	11	{1, 1, 1}	13.946 438 1126/7	$\mathbb{S}_8^-/\mathbb{S}_8^+$
	3.50	12	{0, 2, 1} – {0, 1, 2} – {1, 0, 2} –	14.696 214 3034/6	$\mathbb{S}_2^-/\mathbb{S}_2^+ - \mathbb{S}_3^-/\mathbb{S}_3^+ - \mathbb{S}_4^-/\mathbb{S}_4^+ -$
			{2, 0, 1} – {2, 1, 0} – {1, 2, 0}		$\mathbb{S}_2^-/\mathbb{S}_2^+ - \mathbb{S}_3^-/\mathbb{S}_3^+ - \mathbb{S}_4^-/\mathbb{S}_4^+$
	3.50	12	{0, 0, 3} – {0, 3, 0} – {3, 0, 0}	15.941 507 1808/14	$\mathbb{S}_2^-/\mathbb{S}_2^+ - \mathbb{S}_3^-/\mathbb{S}_3^+ - \mathbb{S}_4^-/\mathbb{S}_4^+$
1	3.25	11	{0, 0, 0}	4.648 812 704 17/25	$\mathbb{S}_1^-/\mathbb{S}_1^+$
	3.35	11	{0, 0, 1} – {0, 1, 0} – {1, 0, 0}	8.380 342 530 07/13	$\mathbb{S}_2^-/\mathbb{S}_2^+ - \mathbb{S}_3^-/\mathbb{S}_3^+ - \mathbb{S}_4^-/\mathbb{S}_4^+$
	3.30	11	{1, 1, 0} – {1, 0, 1} – {0, 1, 1} –	12.485 556 0509/11	$\mathbb{S}_5^-/\mathbb{S}_5^+ - \mathbb{S}_6^-/\mathbb{S}_6^+ - \mathbb{S}_7^-/\mathbb{S}_7^+ -$
			{0, 0, 2} – {0, 2, 0}		$\mathbb{S}_1^-/\mathbb{S}_1^+ - \mathbb{S}_1^-/\mathbb{S}_1^+$
	3.35	11	{2, 0, 0}	13.156 803 8977/84	$\mathbb{S}_1^-/\mathbb{S}_1^+$
	3.45	11	{0, 2, 1} – {0, 1, 2} – {1, 0, 2} –		$\mathbb{S}_2^-/\mathbb{S}_2^+ - \mathbb{S}_3^-/\mathbb{S}_3^+ - \mathbb{S}_4^-/\mathbb{S}_4^+ -$
			{1, 1, 1} –	16.904 036 7034/6	$\mathbb{S}_8^-/\mathbb{S}_8^+ -$
			{2, 0, 1} – {2, 1, 0} – {1, 2, 0}		$\mathbb{S}_2^-/\mathbb{S}_2^+ - \mathbb{S}_3^-/\mathbb{S}_3^+ - \mathbb{S}_4^-/\mathbb{S}_4^+$
	3.45	11	{0, 0, 3} – {0, 3, 0} – {3, 0, 0}	17.861 796 9003/5	$\mathbb{S}_2^-/\mathbb{S}_2^+ - \mathbb{S}_3^-/\mathbb{S}_3^+ - \mathbb{S}_4^-/\mathbb{S}_4^+$
	3.35	11	{1, 1, 2} – {1, 2, 1} – {2, 1, 1} –		$\mathbb{S}_5^-/\mathbb{S}_5^+ - \mathbb{S}_6^-/\mathbb{S}_6^+ - \mathbb{S}_7^-/\mathbb{S}_7^+ -$
			{0, 2, 2} – {2, 0, 2} – {2, 2, 0} –	21.595 037 5740/5	$\mathbb{S}_1^-/\mathbb{S}_1^+ - \mathbb{S}_1^-/\mathbb{S}_1^+ - \mathbb{S}_1^-/\mathbb{S}_1^+ -$
			{1, 3, 0} – {3, 0, 1} – {0, 3, 1}		$\mathbb{S}_5^-/\mathbb{S}_5^+ - \mathbb{S}_6^-/\mathbb{S}_6^+ - \mathbb{S}_7^-/\mathbb{S}_7^+$
10	3.12	13	{0, 0, 0}	6.783 741 257 79/81	$\mathbb{S}_1^-/\mathbb{S}_1^+$
	3.14	13	{0, 0, 1} – {0, 1, 0} – {1, 0, 0}	12.372 384 1382/4	$\mathbb{S}_2^-/\mathbb{S}_2^+ - \mathbb{S}_3^-/\mathbb{S}_3^+ - \mathbb{S}_4^-/\mathbb{S}_4^+$
	3.14	13	{0, 0, 2} – {0, 2, 0}	17.135 018 7447/69	$\mathbb{S}_1^-/\mathbb{S}_1^+ - \mathbb{S}_1^-/\mathbb{S}_1^+$
	3.14	13	{2, 0, 0}	19.340 247 7243/93	$\mathbb{S}_1^-/\mathbb{S}_1^+$
	3.00	13	{1, 1, 0} – {1, 0, 1} – {0, 1, 1}	19.700 467 4037/9	$\mathbb{S}_5^-/\mathbb{S}_5^+ - \mathbb{S}_6^-/\mathbb{S}_6^+ - \mathbb{S}_7^-/\mathbb{S}_7^+$
	3.19	13	{0, 2, 1} – {0, 1, 2} – {1, 0, 2}	22.955 428 3856/83	$\mathbb{S}_2^-/\mathbb{S}_2^+ - \mathbb{S}_3^-/\mathbb{S}_3^+ - \mathbb{S}_4^-/\mathbb{S}_4^+$
	3.07	13	{2, 0, 1} – {2, 1, 0} – {1, 2, 0}	26.102 785 9695/7	$\mathbb{S}_2^-/\mathbb{S}_2^+ - \mathbb{S}_3^-/\mathbb{S}_3^+ - \mathbb{S}_4^-/\mathbb{S}_4^+$
	3.21	13	{0, 0, 3} – {0, 3, 0} – {3, 0, 0}	27.721 566 3968/87	$\mathbb{S}_2^-/\mathbb{S}_2^+ - \mathbb{S}_3^-/\mathbb{S}_3^+ - \mathbb{S}_4^-/\mathbb{S}_4^+$
	2.85	12	{1, 1, 1}	27.996 375 3308/12	$\mathbb{S}_8^-/\mathbb{S}_8^+$

Therefore, we tabulate the lower and upper bound eigenvalues of (3.5) in tables (6), (7) and (8) for c_6 values of 10^{-3}, 1 and 10^3, respectively. Each table includes a set of β and γ parameters, such that

$$(\beta, \gamma) : \{(\tfrac{1}{6}, -1), (1, -1), (10, -1), (\tfrac{1}{6}, 0), (0, 0), (1, 0), (\tfrac{1}{3}, 1), (0, 1), (1, 1)\} \qquad (3.8)$$

satisfying (3.6) and (3.7). Tables 3–8 also contain the quantum numbers $\{n_1,\ n_2,\ n_3\}$ of the energy levels and their respective basis sets, the truncation order N of the wavefunctions and the critical confinement $\ell_{\rm cr}$, at which the desired accuracy is obtained.

Table 5. Lower and upper bounds to the eigenvalues of the quartic oscillator in (3.3), where $c_4 = 10^3$, as a function of α.

α	$\ell_{\rm cr}$	N	$\{n_1,\, n_2,\, n_3\}$	$E_{n_1n_2n_3}$	Basis set
$-\frac{1}{2}$	1.40	14	$\{0,0,0\}$	26.954 388 8412/3	$\mathbb{S}_1^-/\mathbb{S}_1^+$
	1.32	13	$\{0,0,1\}-\{0,1,0\}-\{1,0,0\}$	48.622 258 5030/5	$\mathbb{S}_2^-/\mathbb{S}_2^+-\mathbb{S}_3^-/\mathbb{S}_3^+-\mathbb{S}_4^-/\mathbb{S}_4^+$
	1.36	13	$\{1,1,0\}-\{1,0,1\}-\{0,1,1\}$	65.313 429 3010/43	$\mathbb{S}_5^-/\mathbb{S}_5^+-\mathbb{S}_6^-/\mathbb{S}_6^+-\mathbb{S}_7^-/\mathbb{S}_7^+$
	1.40	14	$\{0,0,2\}$	72.158 150 8000/15	$\mathbb{S}_1^-/\mathbb{S}_1^+$
	1.42	14	$\{1,1,1\}$	76.325 687 7301/29	$\mathbb{S}_8^-/\mathbb{S}_8^+$
	1.44	14	$\{0,2,1\}-\{0,1,2\}-\{1,0,2\}$	85.419 545 0627/73	$\mathbb{S}_2^-/\mathbb{S}_2^+-\mathbb{S}_3^-/\mathbb{S}_3^+-\mathbb{S}_4^-/\mathbb{S}_4^+$
	1.39	14	$\{0,2,0\}-\{2,0,0\}$	85.518 934 5802/20	$\mathbb{S}_1^-/\mathbb{S}_1^+-\mathbb{S}_1^-/\mathbb{S}_1^+$
	1.47	14	$\{1,1,2\}-\{1,2,1\}-\{2,1,1\}$	96.389 107 1032/51	$\mathbb{S}_5^-/\mathbb{S}_5^+-\mathbb{S}_6^-/\mathbb{S}_6^+-\mathbb{S}_7^-/\mathbb{S}_7^+$
	1.44	14	$\{0,2,2\}$	101.767 899 052/116	$\mathbb{S}_1^-/\mathbb{S}_1^+$
	1.28	13	$\{2,0,1\}-\{2,1,0\}-\{1,2,0\}$	101.977 458 650/5	$\mathbb{S}_2^-/\mathbb{S}_2^+-\mathbb{S}_3^-/\mathbb{S}_3^+-\mathbb{S}_4^-/\mathbb{S}_4^+$
0	1.13	12	$\{0,0,0\}$	31.919 366 1339/40	$\mathbb{S}_1^-/\mathbb{S}_1^+$
	1.12	12	$\{0,0,1\}-\{0,1,0\}-\{1,0,0\}$	59.366 410 8819/22	$\mathbb{S}_2^-/\mathbb{S}_2^+-\mathbb{S}_3^-/\mathbb{S}_3^+-\mathbb{S}_4^-/\mathbb{S}_4^+$
	1.12	12	$\{1,1,0\}-\{1,0,1\}-\{0,1,1\}$	86.813 455 6299/303	$\mathbb{S}_5^-/\mathbb{S}_5^+-\mathbb{S}_6^-/\mathbb{S}_6^+-\mathbb{S}_7^-/\mathbb{S}_7^+$
	1.13	12	$\{0,0,2\}-\{0,2,0\}-\{2,0,0\}$	95.960 981 6227/31	$\mathbb{S}_1^-/\mathbb{S}_1^+-\mathbb{S}_1^-/\mathbb{S}_1^+-\mathbb{S}_1^-/\mathbb{S}_1^+$
	1.10	11	$\{1,1,1\}$	114.260 500 377/9	$\mathbb{S}_8^-/\mathbb{S}_8^+$
	1.12	12	$\{0,2,1\}-\{0,1,2\}-\{1,0,2\}-$	123.408 026 370/2	$\mathbb{S}_2^-/\mathbb{S}_2^+-\mathbb{S}_3^-/\mathbb{S}_3^+-\mathbb{S}_4^-/\mathbb{S}_4^+-$
			$\{2,0,1\}-\{2,1,0\}-\{1,2,0\}$		$\mathbb{S}_2^-/\mathbb{S}_2^+-\mathbb{S}_3^-/\mathbb{S}_3^+-\mathbb{S}_4^-/\mathbb{S}_4^+$
	1.12	12	$\{0,0,3\}-\{0,3,0\}-\{3,0,0\}$	137.882 776 355/65	$\mathbb{S}_2^-/\mathbb{S}_2^+-\mathbb{S}_3^-/\mathbb{S}_3^+-\mathbb{S}_4^-/\mathbb{S}_4^+$
1	1.10	11	$\{0,0,0\}$	38.086 833 4593/4	$\mathbb{S}_1^-/\mathbb{S}_1^+$
	1.10	11	$\{0,0,1\}-\{0,1,0\}-\{1,0,0\}$	71.217 716 6315/7	$\mathbb{S}_2^-/\mathbb{S}_2^+-\mathbb{S}_3^-/\mathbb{S}_3^+-\mathbb{S}_4^-/\mathbb{S}_4^+$
	1.10	11	$\{1,1,0\}-\{1,0,1\}-\{0,1,1\}-$	108.595 258 738/9	$\mathbb{S}_5^-/\mathbb{S}_5^+-\mathbb{S}_6^-/\mathbb{S}_6^+-\mathbb{S}_7^-/\mathbb{S}_7^+-$
			$\{0,0,2\}-\{0,2,0\}$		$\mathbb{S}_1^-/\mathbb{S}_1^+-\mathbb{S}_1^-/\mathbb{S}_1^+$
	1.10	11	$\{2,0,0\}$	116.603 198 937/8	$\mathbb{S}_1^-/\mathbb{S}_1^+$
	1.10	11	$\{0,2,1\}-\{0,1,2\}-\{1,0,2\}-$		$\mathbb{S}_2^-/\mathbb{S}_2^+-\mathbb{S}_3^-/\mathbb{S}_3^+-\mathbb{S}_4^-/\mathbb{S}_4^+-$
			$\{1,1,1\}-$	149.439 045 580/1	$\mathbb{S}_8^-/\mathbb{S}_8^+-$
			$\{2,0,1\}-\{2,1,0\}-\{1,2,0\}$		$\mathbb{S}_2^-/\mathbb{S}_2^+-\mathbb{S}_3^-/\mathbb{S}_3^+-\mathbb{S}_4^-/\mathbb{S}_4^+$
	1.12	12	$\{0,0,3\}-\{0,3,0\}-\{3,0,0\}$	160.514 558 044/7	$\mathbb{S}_2^-/\mathbb{S}_2^+-\mathbb{S}_3^-/\mathbb{S}_3^+-\mathbb{S}_4^-/\mathbb{S}_4^+$
	1.10	11	$\{1,1,2\}-\{1,2,1\}-\{2,1,1\}-$		$\mathbb{S}_5^-/\mathbb{S}_5^+-\mathbb{S}_6^-/\mathbb{S}_6^+-\mathbb{S}_7^-/\mathbb{S}_7^+-$
			$\{0,2,2\}-\{2,0,2\}-\{2,2,0\}-$	193.248 820 645/6	$\mathbb{S}_1^-/\mathbb{S}_1^+-\mathbb{S}_1^-/\mathbb{S}_1^+-\mathbb{S}_1^-/\mathbb{S}_1^+-$
			$\{1,3,0\}-\{3,0,1\}-\{0,1,3\}$		$\mathbb{S}_5^-/\mathbb{S}_5^+-\mathbb{S}_6^-/\mathbb{S}_6^+-\mathbb{S}_7^-/\mathbb{S}_7^+$
10	0.96	12	$\{0,0,0\}$	62.444 077 5617/50	$\mathbb{S}_1^-/\mathbb{S}_1^+$
	1.02	14	$\{0,0,1\}-\{0,1,0\}-\{1,0,0\}$	115.453 232 019/21	$\mathbb{S}_2^-/\mathbb{S}_2^+-\mathbb{S}_3^-/\mathbb{S}_3^+-\mathbb{S}_4^-/\mathbb{S}_4^+$
	1.01	14	$\{0,0,2\}-\{0,2,0\}$	159.492 179 901/31	$\mathbb{S}_1^-/\mathbb{S}_1^+-\mathbb{S}_1^-/\mathbb{S}_1^+$
	1.01	14	$\{2,0,0\}$	182.424 212 632/701	$\mathbb{S}_1^-/\mathbb{S}_1^+$
	0.93	12	$\{1,1,0\}-\{1,0,1\}-\{0,1,1\}$	187.200 352 824/36	$\mathbb{S}_5^-/\mathbb{S}_5^+-\mathbb{S}_6^-/\mathbb{S}_6^+-\mathbb{S}_7^-/\mathbb{S}_7^+$
	1.03	14	$\{0,2,1\}-\{0,1,2\}-\{1,0,2\}$	214.929 362 459/535	$\mathbb{S}_2^-/\mathbb{S}_2^+-\mathbb{S}_3^-/\mathbb{S}_3^+-\mathbb{S}_4^-/\mathbb{S}_4^+$
	1.02	14	$\{2,0,1\}-\{2,1,0\}-\{1,2,0\}$	248.733 089 900/4	$\mathbb{S}_2^-/\mathbb{S}_2^+-\mathbb{S}_3^-/\mathbb{S}_3^+-\mathbb{S}_4^-/\mathbb{S}_4^+$
	1.03	14	$\{0,0,3\}-\{0,3,0\}-\{3,0,0\}$	265.057 585 588/668	$\mathbb{S}_2^-/\mathbb{S}_2^+-\mathbb{S}_3^-/\mathbb{S}_3^+-\mathbb{S}_4^-/\mathbb{S}_4^+$
	0.90	12	$\{1,1,1\}$	268.739 781 544/52	$\mathbb{S}_8^-/\mathbb{S}_8^+$

4. Discussion

In this paper, an extensive numerical analysis of three-dimensional anharmonic oscillators is presented via the confined system which generates converging eigenvalue bounds. Tables 1 and 2 exhibit evidently the typical aspects of the method. First, the method can be applied equally well to the quartic and sextic oscillators. Second, the accuracy of the results can be improved by increasing appropriately the boundary parameter ℓ. Furthermore, it is deduced from tables 3–8 that there is no accuracy loss in a very wide range of the

Table 6. Lower and upper bounds to the eigenvalues of the sextic oscillator in (3.5), where $c_6 = 10^{-3}$, as a function of β and γ.

γ	β	ℓ_{cr}	N	$\{n_1,\ n_2,\ n_3\}$	$E_{n_1n_2n_3}$	Basis set
-1	$\frac{1}{6}$	5.50	11	$\{0,0,0\}$	3.005 910 711 55/6	$\mathbb{S}_1^-/\mathbb{S}_1^+$
		5.50	11	$\{0,0,1\}-\{0,1,0\}-\{1,0,0\}$	5.017 549 679 05/6	$\mathbb{S}_2^-/\mathbb{S}_2^+-\mathbb{S}_3^-/\mathbb{S}_3^+-\mathbb{S}_4^-/\mathbb{S}_4^+$
		5.50	11	$\{1,1,0\}-\{1,0,1\}-\{0,1,1\}$	7.029 143 013 81/3	$\mathbb{S}_5^-/\mathbb{S}_5^+-\mathbb{S}_6^-/\mathbb{S}_6^+-\mathbb{S}_7^-/\mathbb{S}_7^+$
		5.50	11	$\{0,0,2\}$	7.051 584 425 35/8	$\mathbb{S}_1^-/\mathbb{S}_1^+$
	1	5.25	10	$\{0,0,0\}$	3.011 350 229 49/50	$\mathbb{S}_1^-/\mathbb{S}_1^+$
		5.50	11	$\{0,0,1\}-\{0,1,0\}-\{1,0,0\}$	5.033 558 556 88/9	$\mathbb{S}_2^-/\mathbb{S}_2^+-\mathbb{S}_3^-/\mathbb{S}_3^+-\mathbb{S}_4^-/\mathbb{S}_4^+$
		5.50	11	$\{1,1,0\}-\{1,0,1\}-\{0,1,1\}$	7.069 304 041 10/1	$\mathbb{S}_5^-/\mathbb{S}_5^+-\mathbb{S}_6^-/\mathbb{S}_6^+-\mathbb{S}_7^-/\mathbb{S}_7^+$
		5.50	11	$\{0,0,2\}-\{0,2,0\}$	7.077 436 038 17/20	$\mathbb{S}_1^-/\mathbb{S}_1^+-\mathbb{S}_1^-/\mathbb{S}_1^+$
	10	5.00	10	$\{0,0,0\}$	3.063 696 942 56/7	$\mathbb{S}_1^-/\mathbb{S}_1^+$
		5.25	11	$\{0,0,1\}-\{0,1,0\}-\{1,0,0\}$	5.178 879 727 96/7	$\mathbb{S}_2^-/\mathbb{S}_2^+-\mathbb{S}_3^-/\mathbb{S}_3^+-\mathbb{S}_4^-/\mathbb{S}_4^+$
		5.25	11	$\{1,1,0\}-\{1,0,1\}-\{0,1,1\}$	7.409 006 072 14/5	$\mathbb{S}_5^-/\mathbb{S}_5^+-\mathbb{S}_6^-/\mathbb{S}_6^+-\mathbb{S}_7^-/\mathbb{S}_7^+$
		5.25	11	$\{0,0,2\}-\{0,2,0\}$	7.304 657 341 01/7	$\mathbb{S}_1^-/\mathbb{S}_1^+-\mathbb{S}_1^-/\mathbb{S}_1^+$
0	$-\frac{1}{6}$	5.25	10	$\{0,0,0\}$	3.004 440 819 29/30	$\mathbb{S}_1^-/\mathbb{S}_1^+$
		5.50	11	$\{0,0,1\}-\{0,1,0\}-\{1,0,0\}$	5.013 191 576 00/1	$\mathbb{S}_2^-/\mathbb{S}_2^+-\mathbb{S}_3^-/\mathbb{S}_3^+-\mathbb{S}_4^-/\mathbb{S}_4^+$
		5.50	11	$\{1,1,0\}-\{1,0,1\}-\{0,1,1\}$	7.019 056 729 05/6	$\mathbb{S}_5^-/\mathbb{S}_5^+-\mathbb{S}_6^-/\mathbb{S}_6^+-\mathbb{S}_7^-/\mathbb{S}_7^+$
		5.50	11	$\{0,0,2\}$	7.038 763 575 82/6	$\mathbb{S}_1^-/\mathbb{S}_1^+$
	0	5.25	10	$\{0,0,0\}$	3.005 546 446 71/2	$\mathbb{S}_1^-/\mathbb{S}_1^+$
		5.25	10	$\{0,0,1\}-\{0,1,0\}-\{1,0,0\}$	5.016 478 591 81/6	$\mathbb{S}_2^-/\mathbb{S}_2^+-\mathbb{S}_3^-/\mathbb{S}_3^+-\mathbb{S}_4^-/\mathbb{S}_4^+$
		5.50	11	$\{1,1,0\}-\{1,0,1\}-\{0,1,1\}$	7.027 410 736 95/6	$\mathbb{S}_5^-/\mathbb{S}_5^+-\mathbb{S}_6^-/\mathbb{S}_6^+-\mathbb{S}_7^-/\mathbb{S}_7^+$
		5.50	11	$\{0,0,2\}-\{0,2,0\}-\{2,0,0\}$	7.048 497 556 91/5	$\mathbb{S}_1^-/\mathbb{S}_1^+-\mathbb{S}_1^-/\mathbb{S}_1^+-\mathbb{S}_1^-/\mathbb{S}_1^+$
	1	5.25	10	$\{0,0,0\}$	3.012 067 327 00/1	$\mathbb{S}_1^-/\mathbb{S}_1^+$
		5.25	11	$\{0,0,1\}-\{0,1,0\}-\{1,0,0\}$	5.035 655 952 21/2	$\mathbb{S}_2^-/\mathbb{S}_2^+-\mathbb{S}_3^-/\mathbb{S}_3^+-\mathbb{S}_4^-/\mathbb{S}_4^+$
		5.50	11	$\{1,1,0\}-\{1,0,1\}-\{0,1,1\}$	7.075 424 338 37/8	$\mathbb{S}_5^-/\mathbb{S}_5^+-\mathbb{S}_6^-/\mathbb{S}_6^+-\mathbb{S}_7^-/\mathbb{S}_7^+$
		5.50	11	$\{0,0,2\}-\{0,2,0\}$	7.079 454 939 54/6	$\mathbb{S}_1^-/\mathbb{S}_1^+-\mathbb{S}_1^-/\mathbb{S}_1^+$
1	$-\frac{1}{3}$	5.25	10	$\{0,0,0\}$	3.004 073 434 18/9	$\mathbb{S}_1^-/\mathbb{S}_1^+$
		5.50	11	$\{0,0,1\}-\{0,1,0\}-\{1,0,0\}$	5.012 104 761 21/2	$\mathbb{S}_2^-/\mathbb{S}_2^+-\mathbb{S}_3^-/\mathbb{S}_3^+-\mathbb{S}_4^-/\mathbb{S}_4^+$
		5.50	11	$\{1,1,0\}-\{1,0,1\}-\{0,1,1\}$	7.017 267 137 97/9	$\mathbb{S}_5^-/\mathbb{S}_5^+-\mathbb{S}_6^-/\mathbb{S}_6^+-\mathbb{S}_7^-/\mathbb{S}_7^+$
		5.50	11	$\{0,0,2\}$	7.035 591 531 67/71	$\mathbb{S}_1^-/\mathbb{S}_1^+$
	0	5.25	10	$\{0,0,0\}$	3.006 282 320 43/5	$\mathbb{S}_1^-/\mathbb{S}_1^+$
		5.50	11	$\{0,0,1\}-\{0,1,0\}-\{1,0,0\}$	5.018 666 315 27/8	$\mathbb{S}_2^-/\mathbb{S}_2^+-\mathbb{S}_3^-/\mathbb{S}_3^+-\mathbb{S}_4^-/\mathbb{S}_4^+$
		5.50	11	$\{1,1,0\}-\{1,0,1\}-\{0,1,1\}$	7.033 906 257 68/9	$\mathbb{S}_5^-/\mathbb{S}_5^+-\mathbb{S}_6^-/\mathbb{S}_6^+-\mathbb{S}_7^-/\mathbb{S}_7^+$
		5.50	11	$\{0,0,2\}-\{0,2,0\}$	7.050 636 386 05/8	$\mathbb{S}_1^-/\mathbb{S}_1^+-\mathbb{S}_1^-/\mathbb{S}_1^+$
	1	5.25	10	$\{0,0,0\}$	3.012 780 960 68/70	$\mathbb{S}_1^-/\mathbb{S}_1^+$
		5.25	10	$\{0,0,1\}-\{0,1,0\}-\{1,0,0\}$	5.037 735 793 50/3	$\mathbb{S}_2^-/\mathbb{S}_2^+-\mathbb{S}_3^-/\mathbb{S}_3^+-\mathbb{S}_4^-/\mathbb{S}_4^+$
		5.25	10	$\{1,1,0\}-\{1,0,1\}-\{0,1,1\}-$ $\{0,0,2\}-\{0,2,0\}$	7.081 459 967 43/7	$\mathbb{S}_5^-/\mathbb{S}_5^+-\mathbb{S}_6^-/\mathbb{S}_6^+-\mathbb{S}_7^-/\mathbb{S}_7^+-$ $\mathbb{S}_1^-/\mathbb{S}_1^+-\mathbb{S}_1^-/\mathbb{S}_1^+$
		5.50	11	$\{2,0,0\}$	7.110 092 855 85/7	$\mathbb{S}_1^-/\mathbb{S}_1^+$

anharmonicity constants. In fact, a significant property of this class of eigenvalue problems is the existence of two distinct regimes of values of the coupling constants and the quantum numbers. The two regimes are referred to as the nearly harmonic and the nearly pure anharmonic, respectively, for the small and large values of the eigenvalue parameters. It is well known that most of the numerical techniques are efficiently used in one of these regimes. Therefore, the confined system approach makes our method more versatile and applicable with uniform precision to almost any type of Schrödinger potential. We believe that the spectrum of a perturbed three-dimensional Hamiltonian in the present generality is computed for the first time.

Table 7. Lower and upper bounds to the eigenvalues of the sextic oscillator in (3.5), where $c_6 = 1$, as a function of β and γ.

γ	β	ℓ_{cr}	N	$\{n_1, n_2, n_3\}$	$E_{n_1 n_2 n_3}$	Basis set
−1	$\frac{1}{6}$	2.65	12	{0,0,0}	4.34348616268/77	$\mathbb{S}_1^-/\mathbb{S}_1^+$
		2.65	12	{0, 0, 1} − {0, 1, 0} − {1, 0, 0}	7.963 709 078 44/73	$\mathbb{S}_2^-/\mathbb{S}_2^+ - \mathbb{S}_3^-/\mathbb{S}_3^+ - \mathbb{S}_4^-/\mathbb{S}_4^+$
		2.65	12	{1, 1, 0} − {1, 0, 1} − {0, 1, 1}	11.483 804 2150/7	$\mathbb{S}_5^-/\mathbb{S}_5^+ - \mathbb{S}_6^-/\mathbb{S}_6^+ - \mathbb{S}_7^-/\mathbb{S}_7^+$
		2.65	12	{0, 0, 2}	12.825 266 6016/34	$\mathbb{S}_1^-/\mathbb{S}_1^+$
	1	2.65	10	{0, 0, 0}	4.919 667 855 01/2	$\mathbb{S}_1^-/\mathbb{S}_1^+$
		2.65	11	{0, 0, 1} − {0, 1, 0} − {1, 0, 0}	9.218 991 650 08/13	$\mathbb{S}_2^-/\mathbb{S}_2^+ - \mathbb{S}_3^-/\mathbb{S}_3^+ - \mathbb{S}_4^-/\mathbb{S}_4^+$
		2.65	11	{1, 1, 0} − {1, 0, 1} − {0, 1, 1}	14.049 874 035 2/3	$\mathbb{S}_5^-/\mathbb{S}_5^+ - \mathbb{S}_6^-/\mathbb{S}_6^+ - \mathbb{S}_7^-/\mathbb{S}_7^+$
		2.65	11	{0, 0, 2} − {0, 2, 0}	14.416 607 1509/13	$\mathbb{S}_1^-/\mathbb{S}_1^+ - \mathbb{S}_1^-/\mathbb{S}_1^+$
	10	2.45	12	{0, 0, 0}	7.060 561 585 02/6	$\mathbb{S}_1^-/\mathbb{S}_1^+$
		2.45	12	{0, 0, 1} − {0, 1, 0} − {1, 0, 0}	13.465 529 8282/5	$\mathbb{S}_2^-/\mathbb{S}_2^+ - \mathbb{S}_3^-/\mathbb{S}_3^+ - \mathbb{S}_4^-/\mathbb{S}_4^+$
		2.45	12	{0, 0, 2} − {0, 2, 0}	19.782 277 3035/59	$\mathbb{S}_1^-/\mathbb{S}_1^+ - \mathbb{S}_1^-/\mathbb{S}_1^+$
		2.38	12	{1, 1, 0} − {1, 0, 1} − {0, 1, 1}	21.803 623 6197/9	$\mathbb{S}_5^-/\mathbb{S}_5^+ - \mathbb{S}_6^-/\mathbb{S}_6^+ - \mathbb{S}_7^-/\mathbb{S}_7^+$
0	$-\frac{1}{6}$	2.70	12	{0, 0, 0}	4.116 458 109 02/21	$\mathbb{S}_1^-/\mathbb{S}_1^+$
		2.77	12	{0, 0, 1} − {0, 1, 0} − {1, 0, 0}	7.447 129 679 96/9	$\mathbb{S}_2^-/\mathbb{S}_2^+ - \mathbb{S}_3^-/\mathbb{S}_3^+ - \mathbb{S}_4^-/\mathbb{S}_4^+$
		2.77	12	{1, 1, 0} − {1, 0, 1} − {0, 1, 1}	10.509 404 8479/93	$\mathbb{S}_5^-/\mathbb{S}_5^+ - \mathbb{S}_6^-/\mathbb{S}_6^+ - \mathbb{S}_7^-/\mathbb{S}_7^+$
		2.77	12	{0, 0, 2}	11.680 031 8516/46	$\mathbb{S}_1^-/\mathbb{S}_1^+$
	0	2.65	12	{0, 0, 0}	4.306 873 856 95/708	$\mathbb{S}_1^-/\mathbb{S}_1^+$
		2.65	12	{0, 0, 1} − {0, 1, 0} − {1, 0, 0}	7.904 645 175 51/95	$\mathbb{S}_2^-/\mathbb{S}_2^+ - \mathbb{S}_3^-/\mathbb{S}_3^+ - \mathbb{S}_4^-/\mathbb{S}_4^+$
		2.65	12	{1, 1, 0} − {1, 0, 1} − {0, 1, 1}	1.502 416 4940/9	$\mathbb{S}_5^-/\mathbb{S}_5^+ - \mathbb{S}_6^-/\mathbb{S}_6^+ - \mathbb{S}_7^-/\mathbb{S}_7^+$
		2.65	12	{0, 0, 2} − {0, 2, 0} − {2, 0, 0}	12.837 871 2370/90	$\mathbb{S}_1^-/\mathbb{S}_1^+ - \mathbb{S}_1^-/\mathbb{S}_1^+ - \mathbb{S}_1^-/\mathbb{S}_1^+$
	1	2.61	12	{0, 0, 0}	4.978 778 995 16/22	$\mathbb{S}_1^-/\mathbb{S}_1^+$
		2.63	12	{0, 0, 1} − {0, 1, 0} − {1, 0, 0}	9.343 189 699 39/49	$\mathbb{S}_2^-/\mathbb{S}_2^+ - \mathbb{S}_3^-/\mathbb{S}_3^+ - \mathbb{S}_4^-/\mathbb{S}_4^+$
		2.61	12	{1, 1, 0} − {1, 0, 1} − {0, 1, 1}	14.333 715 2290/2	$\mathbb{S}_5^-/\mathbb{S}_5^+ - \mathbb{S}_6^-/\mathbb{S}_6^+ - \mathbb{S}_7^-/\mathbb{S}_7^+$
		2.61	12	{0, 0, 2} − {0, 2, 0}	14.502 895 9025/41	$\mathbb{S}_1^-/\mathbb{S}_1^+ - \mathbb{S}_1^-/\mathbb{S}_1^+$
1	$-\frac{1}{3}$	2.82	12	{0, 0, 0}	4.062 464 558 41/93	$\mathbb{S}_1^-/\mathbb{S}_1^+$
		2.89	12	{0, 0, 1} − {0, 1, 0} − {1, 0, 0}	7.342 831 040 38/75	$\mathbb{S}_2^-/\mathbb{S}_2^+ - \mathbb{S}_3^-/\mathbb{S}_3^+ - \mathbb{S}_4^-/\mathbb{S}_4^+$
		2.94	12	{1, 1, 0} − {1, 0, 1} − {0, 1, 1}	10.436 511 4346/55	$\mathbb{S}_5^-/\mathbb{S}_5^+ - \mathbb{S}_6^-/\mathbb{S}_6^+ - \mathbb{S}_7^-/\mathbb{S}_7^+$
		2.91	12	{0, 0, 2}	11.566 697 0923/59	$\mathbb{S}_1^-/\mathbb{S}_1^+$
	0	2.63	12	{0, 0, 0}	4.417 241 165 94/613	$\mathbb{S}_1^-/\mathbb{S}_1^+$
		2.63	12	{0, 0, 1} − {0, 1, 0} − {1, 0, 0}	8.161 819 733 17/86	$\mathbb{S}_2^-/\mathbb{S}_2^+ - \mathbb{S}_3^-/\mathbb{S}_3^+ - \mathbb{S}_4^-/\mathbb{S}_4^+$
		2.63	12	{1, 1, 0} − {1, 0, 1} − {0, 1, 1}	12.100 307 6520/30	$\mathbb{S}_5^-/\mathbb{S}_5^+ - \mathbb{S}_6^-/\mathbb{S}_6^+ - \mathbb{S}_7^-/\mathbb{S}_7^+$
		2.63	12	{0, 0, 2} − {0, 2, 0}	13.016 318 2262/97	$\mathbb{S}_1^-/\mathbb{S}_1^+ - \mathbb{S}_1^-/\mathbb{S}_1^+$
	1	2.62	12	{0, 0, 0}	5.033 395 937 70/4	$\mathbb{S}_1^-/\mathbb{S}_1^+$
		2.62	12	{0, 0, 1} − {0, 1, 0} − {1, 0, 0}	9.455 535 276 77/91	$\mathbb{S}_2^-/\mathbb{S}_2^+ - \mathbb{S}_3^-/\mathbb{S}_3^+ - \mathbb{S}_4^-/\mathbb{S}_4^+$
		2.62	12	{1, 1, 0} − {1, 0, 1} − {0, 1, 1} − {0, 0, 2} − {0, 2, 0}	14.584 132 9457/8	$\mathbb{S}_5^-/\mathbb{S}_5^+ - \mathbb{S}_6^-/\mathbb{S}_6^+ - \mathbb{S}_7^-/\mathbb{S}_7^+ - \mathbb{S}_1^-/\mathbb{S}_1^+ - \mathbb{S}_1^-/\mathbb{S}_1^+$
		2.62	12	{2, 0, 0}	15.989 440 7874/84	$\mathbb{S}_1^-/\mathbb{S}_1^+$

The crucial point of our approximation lies in the determination of a critical confinement size denoted by ℓ_{cr}, to achieve satisfactory results. We infer that this depends mainly on the dominant terms of the potential function and the quantum numbers of the state being considered. It is noteworthy that the required ℓ_{cr} values can be estimated roughly after a few computer experiments. As a matter of fact, it is unnecessary to find these values very precisely since the accuracy of the results is virtually the same in the near vicinity of a specific confinement. Obviously, because both lower and upper bounds are calculated simultaneously for a predicted ℓ_{cr}, there is no uncertainty in the tabulated eigenvalues. Hence, the numerical evaluations support completely the theoretical analysis in the appendix.

Table 8. Lower and upper bounds to the eigenvalues of the sextic oscillator in (3.5), where $c_6 = 10^3$, as a function of β and γ.

γ	β	ℓ_{cr}	N	$\{n_1, n_2, n_3\}$	$E_{n_1n_2n_3}$	Basis set
−1	$\frac{1}{6}$	1.13	12	{0, 0, 0}	19.713 219 4856/62	$\mathbb{S}_1^-/\mathbb{S}_1^+$
		1.14	12	{0, 0, 1} − {0, 1, 0} − {1, 0, 0}	37.806 450 8817/22	$\mathbb{S}_2^-/\mathbb{S}_2^+ - \mathbb{S}_3^-/\mathbb{S}_3^+ - \mathbb{S}_4^-/\mathbb{S}_4^+$
		1.14	12	{1, 1, 0} − {1, 0, 1} − {0, 1, 1}	55.066 790 5505/47	$\mathbb{S}_5^-/\mathbb{S}_5^+ - \mathbb{S}_6^-/\mathbb{S}_6^+ - \mathbb{S}_7^-/\mathbb{S}_7^+$
		1.15	13	{0, 0, 2}	63.491 336 8818/84	$\mathbb{S}_1^-/\mathbb{S}_1^+$
	1	1.10	12	{0, 0, 0}	23.769 236 2930/6	$\mathbb{S}_1^-/\mathbb{S}_1^+$
		1.12	11	{0, 0, 1} − {0, 1, 0} − {1, 0, 0}	46.277 484 0394/415	$\mathbb{S}_2^-/\mathbb{S}_2^+ - \mathbb{S}_3^-/\mathbb{S}_3^+ - \mathbb{S}_4^-/\mathbb{S}_4^+$
		1.10	12	{1, 1, 0} − {1, 0, 1} − {0, 1, 1}	71.995 675 5242/9	$\mathbb{S}_5^-/\mathbb{S}_5^+ - \mathbb{S}_6^-/\mathbb{S}_6^+ - \mathbb{S}_7^-/\mathbb{S}_7^+$
		1.11	12	{0, 0, 2} − {0, 2, 0}	74.282 190 3355/414	$\mathbb{S}_1^-/\mathbb{S}_1^+ - \mathbb{S}_1^-/\mathbb{S}_1^+$
	10	1.03	12	{0, 0, 0}	37.148 422 8147/55	$\mathbb{S}_1^-/\mathbb{S}_1^+$
		1.03	12	{0, 0, 1} − {0, 1, 0} − {1, 0, 0}	72.048 647 7728/76	$\mathbb{S}_2^-/\mathbb{S}_2^+ - \mathbb{S}_3^-/\mathbb{S}_3^+ - \mathbb{S}_4^-/\mathbb{S}_4^+$
		1.03	12	{0, 0, 2} − {0, 2, 0}	106.329 189 226/74	$\mathbb{S}_1^-/\mathbb{S}_1^+ - \mathbb{S}_1^-/\mathbb{S}_1^+$
		1.01	12	{1, 1, 0} − {1, 0, 1} − {0, 1, 1}	118.291 434 651/2	$\mathbb{S}_5^-/\mathbb{S}_5^+ - \mathbb{S}_6^-/\mathbb{S}_6^+ - \mathbb{S}_7^-/\mathbb{S}_7^+$
0	$-\frac{1}{6}$	1.17	12	{0, 0, 0}	17.954 909 8211/25	$\mathbb{S}_1^-/\mathbb{S}_1^+$
		1.19	12	{0, 0, 1} − {0, 1, 0} − {1, 0, 0}	33.995 911 8980/99	$\mathbb{S}_2^-/\mathbb{S}_2^+ - \mathbb{S}_3^-/\mathbb{S}_3^+ - \mathbb{S}_4^-/\mathbb{S}_4^+$
		1.21	12	{1, 1, 0} − {1, 0, 1} − {0, 1, 1}	48.172 283 4377/406	$\mathbb{S}_5^-/\mathbb{S}_5^+ - \mathbb{S}_6^-/\mathbb{S}_6^+ - \mathbb{S}_7^-/\mathbb{S}_7^+$
		1.22	13	{0, 0, 2}	55.381 509 3761/998	$\mathbb{S}_1^-/\mathbb{S}_1^+$
	0	1.15	12	{0, 0, 0}	19.477 050 3970/3	$\mathbb{S}_1^-/\mathbb{S}_1^+$
		1.15	12	{0, 0, 1} − {0, 1, 0} − {1, 0, 0}	37.510 016 3517/20	$\mathbb{S}_2^-/\mathbb{S}_2^+ - \mathbb{S}_3^-/\mathbb{S}_3^+ - \mathbb{S}_4^-/\mathbb{S}_4^+$
		1.15	12	{1, 1, 0} − {1, 0, 1} − {0, 1, 1}	55.542 982 3064/7	$\mathbb{S}_5^-/\mathbb{S}_5^+ - \mathbb{S}_6^-/\mathbb{S}_6^+ - \mathbb{S}_7^-/\mathbb{S}_7^+$
		1.15	12	{0, 0, 2} − {0, 2, 0} − {2, 0, 0}	64.167 180 3713/74	$\mathbb{S}_1^-/\mathbb{S}_1^+ - \mathbb{S}_1^-/\mathbb{S}_1^+ - \mathbb{S}_1^-/\mathbb{S}_1^+$
	1	1.12	12	{0, 0, 0}	24.164 292 6621/3	$\mathbb{S}_1^-/\mathbb{S}_1^+$
		1.12	12	{0, 0, 1} − {0, 1, 0} − {1, 0, 0}	47.073 279 1739/43	$\mathbb{S}_2^-/\mathbb{S}_2^+ - \mathbb{S}_3^-/\mathbb{S}_3^+ - \mathbb{S}_4^-/\mathbb{S}_4^+$
		1.12	12	{1, 1, 0} − {1, 0, 1} − {0, 1, 1}	73.770 465 8095/6	$\mathbb{S}_5^-/\mathbb{S}_5^+ - \mathbb{S}_6^-/\mathbb{S}_6^+ - \mathbb{S}_7^-/\mathbb{S}_7^+$
		1.12	12	{0, 0, 2} − {0, 2, 0}	74.817 379 7500/22	$\mathbb{S}_1^-/\mathbb{S}_1^+ - \mathbb{S}_1^-/\mathbb{S}_1^+$
1	$-\frac{1}{3}$	1.27	13	{0, 0, 0}	17.557 464 6788/99	$\mathbb{S}_1^-/\mathbb{S}_1^+$
		1.27	13	{0, 0, 1} − {0, 1, 0} − {1, 0, 0}	33.342 328 3679/847	$\mathbb{S}_2^-/\mathbb{S}_2^+ - \mathbb{S}_3^-/\mathbb{S}_3^+ - \mathbb{S}_4^-/\mathbb{S}_4^+$
		1.30	13	{1, 1, 0} − {1, 0, 1} − {0, 1, 1}	48.039 135 2733/837	$\mathbb{S}_5^-/\mathbb{S}_5^+ - \mathbb{S}_6^-/\mathbb{S}_6^+ - \mathbb{S}_7^-/\mathbb{S}_7^+$
		1.31	13	{0, 0, 2}	55.229 896 8870/964	$\mathbb{S}_1^-/\mathbb{S}_1^+$
	0	1.15	12	{0, 0, 0}	20.306 232 9130/2	$\mathbb{S}_1^-/\mathbb{S}_1^+$
		1.15	12	{0, 0, 1} − {0, 1, 0} − {1, 0, 0}	39.346 102 7851/2	$\mathbb{S}_2^-/\mathbb{S}_2^+ - \mathbb{S}_3^-/\mathbb{S}_3^+ - \mathbb{S}_4^-/\mathbb{S}_4^+$
		1.14	12	{1, 1, 0} − {1, 0, 1} − {0, 1, 1}	59.615 936 5807/14	$\mathbb{S}_5^-/\mathbb{S}_5^+ - \mathbb{S}_6^-/\mathbb{S}_6^+ - \mathbb{S}_7^-/\mathbb{S}_7^+$
		1.15	12	{0, 0, 2} − {0, 2, 0}	65.380 914 7609/59	$\mathbb{S}_1^-/\mathbb{S}_1^+ - \mathbb{S}_1^-/\mathbb{S}_1^+$
	1	1.12	12	{0, 0, 0}	24.525 316 0869/70	$\mathbb{S}_1^-/\mathbb{S}_1^+$
		1.12	12	{0, 0, 1} − {0, 1, 0} − {1, 0, 0}	47.785 019 8802/6	$\mathbb{S}_2^-/\mathbb{S}_2^+ - \mathbb{S}_3^-/\mathbb{S}_3^+ - \mathbb{S}_4^-/\mathbb{S}_4^+$
		1.12	12	{1, 1, 0} − {1, 0, 1} − {0, 1, 1} − {0, 0, 2} − {0, 2, 0}	75.318 478 6376/7	$\mathbb{S}_5^-/\mathbb{S}_5^+ - \mathbb{S}_6^-/\mathbb{S}_6^+ - \mathbb{S}_7^-/\mathbb{S}_7^+ - \mathbb{S}_1^-/\mathbb{S}_1^+ - \mathbb{S}_1^-/\mathbb{S}_1^+$
		1.12	12	{2, 0, 0}	84.175 583 7757/75	$\mathbb{S}_1^-/\mathbb{S}_1^+$

It is shown from (2.23) that a truncated wavefunction of order N leads to a matrix eigenvalue problem of order N^3. Since the diagonalization of a large matrix is highly time consuming, we content ourselves with a truncation size of about 12 to 13, which yields approximately 12 significant figures accuracy. Certainly, more accurate results can be obtained at the cost of greater computation times. Another remark is that the convergence rates of the Dirichlet and Neumann basis sets in (2.6) and (2.7) are almost equivalent.

For $\alpha = 1$ and $\beta = \gamma = 1$, we have the isotropic quartic and the sextic oscillators, respectively. Therefore, the Schrödinger equation (1.1) can be treated in spherical polar coordinates by the separation of variables proposing a solution of the type $\Psi(r, \theta, \phi) =$

$\mathcal{R}(r)P_l^m(\theta)\,e^{im\phi}$. Here, $P_l^m(\theta)$ with $l \geqslant |m|$ are the associated Legendre functions, and $\mathcal{R}(r)$ satisfies the radial Schrödinger equation

$$\left\{r^2\frac{d^2}{dr^2} + 2r\frac{d}{dr} + r^2[E - V(r)] - l(l+1)\right\}\mathcal{R}(r) = 0. \tag{4.1}$$

In this representation, each energy level is independent of the magnetic quantum number m, $m = 0, \pm 1, \pm 2, \ldots, \pm l$, and thus $(2l+1)$-fold degenerate. The spectrum then contains non-degenerate eigenvalues corresponding to $l = 0$, threefold degenerate eigenvalues corresponding to $l = 1$ and so on. This structure in the spherically symmetric cases can be seen clearly from our tables. However, the computation of the spectrum directly from (4.1) is an ongoing study. In fact, separate and particular research into the radial Schrödinger equation along this line seems to be quite interesting since it bears a different mathematical character.

Another special situation occurs when $\alpha = 0$ and $\beta = \gamma = 0$ for the quartic and sextic perturbations in (3.3) and (3.5), respectively. In these cases the problem reduces to three independent quartic or sextic anharmonic oscillators. As a result, the energy levels are expressible as

$$E_{n_1 n_2 n_3} = E_{n_1} + E_{n_2} + E_{n_3} \tag{4.2}$$

where E_{n_i} $(i = 1, 2, 3)$ denote the eigenvalues of the relevant problem in one dimension. Equation (4.2) implies that the different permutations of a fixed set of quantum numbers $\{n_1, n_2, n_3\}$ indicate the same energy, a property which clarifies the degeneracies of the spectrum of the system. Hence the eigenvalues are either single if $n_1 = n_2 = n_3$ or threefold degenerate if $n_i = n_j \neq n_k$ $(i, j, k = 1, 2, 3)$ or sixfold degenerate if $n_1 \neq n_2 \neq n_3$.

Apart from the particular forms of the potentials, we observe that the mixed parity states are threefold degenerate throughout. These energy levels with two even plus one odd and with one even plus two odd quantum numbers are determined by the sets $\mathbb{S}_2^+$ $(\mathbb{S}_2^-)$, $\mathbb{S}_3^+$ $(\mathbb{S}_3^-)$, $\mathbb{S}_4^+$ $(\mathbb{S}_4^-)$ and $\mathbb{S}_5^+$ $(\mathbb{S}_5^-)$, $\mathbb{S}_6^+$ $(\mathbb{S}_6^-)$, $\mathbb{S}_7^+$ $(\mathbb{S}_7^-)$, respectively. The eigenvalues with the same parity yielded by the sets $\mathbb{S}_1^+$ $(\mathbb{S}_1^-)$ and $\mathbb{S}_8^+$ $(\mathbb{S}_8^-)$ are either single or doubly degenerate in a three-dimensional system. This can easily be attributed to the interchange symmetries of the potential functions considered numerically in this work.

On the other hand, in the case where $\alpha = 0$ and, therefore, (3.3) reduces to three independent quartic oscillators, additional checks on the reliability and consistency of our two-sided bounds are provided by making use of the numerical results of one dimension. Indeed, very accurate eigenvalues are numerically known for $V(x) = x^2 + c_4x^4$ [2, 5], the first three of which, performed in [2] by Banerjee, are listed in table 9. The energy levels determined by the relation (4.2) are then compared in table 10 with the current eigenvalue bounds estimated by the three-dimensional treatment of the problem. Fortunately, the results are in excellent agreement for all states and anharmonicity constants. Moreover, the one-dimensional sextic oscillator Hamiltonian

$$\left(-\frac{d^2}{dx^2} + v_2x^2 + v_4x^4 + v_6x^6\right)\Psi = E\Psi \qquad \lim_{x\to\pm\infty}\Psi(x) = 0 \tag{4.3}$$

is an example of quasi-exactly solvable system provided that suitable algebraic relations between the coupling constants hold. For instance, the ground-state eigenfunction is

$$\Psi_0(x) = e^{-\frac{1}{4}Ax^4 - \frac{1}{2}Bx^2} \qquad A = \sqrt{v_6} > 0 \qquad B = \tfrac{1}{2}v_4v_6^{-1/2} \tag{4.4}$$

with the corresponding energy

$$E_0 = B \tag{4.5}$$

Table 9. The numerically exact eigenvalues of the one-dimensional quartic oscillator $V(x) = x^2 + c_4x^4$, as a function of c_4. Data are taken from [2].

c_4	E_0	E_1	E_2
10^{-3}	1.000 748 692 673	3.003 739 748 168	5.009 711 872 788
1	1.392 351 641 530	4.648 812 704 212	8.655 049 957 759
10^3	10.639 788 711 33	38.086 833 459 38	74.681 404 200 16

Table 10. The comparison of the current eigenvalue bounds for the potential $V(x, y, z) = x^2 + y^2 + z^2 + c_4(x^4 + y^4 + z^4)$ representing three independent quartic oscillators, with results of the one-dimensional case. The results for $E_{n_1} + E_{n_2} + E_{n_3}$ with $n_1, n_2, n_3 = 0, 1, 2$ are calculated from table 9, while those for $E^-_{n_1n_2n_3}$ and $E^+_{n_1n_2n_3}$ stand for the lower and upper bounds, respectively, in our tables 3, 4 and 5, where $\alpha = 0$.

c_4	$\{n_1, n_2, n_3\}$	$E_{n_1} + E_{n_2} + E_{n_3}$	$E^-_{n_1n_2n_3}/E^+_{n_1n_2n_3}$
10^{-3}	{0, 0, 0}	3.002 246 078 019	3.002 246 078 01/3
	{0, 0, 1} – {0, 1, 0} – {1, 0, 0}	5.005 237 133 514	5.005 237 133 51/2
	{1, 1, 0} – {1, 0, 1} – {0, 1, 1}	7.008 228 189 009	7.008 228 189 00/2
	{0, 0, 2} – {0, 2, 0} – {2, 0, 0}	7.011 209 258 134	7.011 209 258 11/6
	{1, 1, 1}	9.011 219 244 504	9.011 219 244 49/53
1	{0, 0, 0}	4.177 054 924 590	4.177 054 924 59/60
	{0, 0, 1} – {0, 1, 0} – {1, 0, 0}	7.433 515 987 272	7.433 515 987 26/9
	{1, 1, 0} – {1, 0, 1} – {0, 1, 1}	10.689 977 049 95	10.689 977 0499/500
	{0, 0, 2} – {0, 2, 0} – {2, 0, 0}	11.439 753 240 82	11.439 753 2407/10
	{1, 1, 1}	13.946 438 112 64	13.946 438 1126/7
10^3	{0, 0, 0}	31.919 366 133 98	31.919 366 1339/40
	{0, 0, 1} – {0, 1, 0} – {1, 0, 0}	59.366 410 882 04	59.366 410 8819/22
	{1, 1, 0} – {1, 0, 1} – {0, 1, 1}	86.813 455 630 09	86.813 455 6299/303
	{0, 0, 2} – {0, 2, 0} – {2, 0, 0}	95.960 981 622 82	95.960 981 6227/31
	{1, 1, 1}	114.260 500 3781	114.260 500 377/9

for the special values of v_2, $v_2 = B^2 - 3A$, as may be verified directly. In particular, for $v_6 = 1$ and $v_4 = 4$ we see that v_2 must be taken as 1 and that $E_0 = 2$. Thus the relation (4.2) now suggests that the lowest eigenvalue of the potential

$$V(x, y, z) = x^2 + y^2 + z^2 + 4(x^4 + y^4 + z^4) + x^6 + y^6 + z^6 \tag{4.6}$$

representing three independent sextic oscillators, can be found analytically such that $E_{0,0,0} = 6$. Table 11 demonstrates the rate of convergence of the lower and upper bounds in this case, as a function of ℓ, which clarifies once more the accuracy of the present method.

In the second special case of the spherically symmetrical potentials for which $a_{m-l,l-k,k} = 1$ for all m, l, k in (1.2), the substitution of $r^2 = x^2 + y^2 + z^2$ transforms $V(x, y, z)$ into a function $V(r)$ of a single variable, i.e.

$$V(r) = \sum_{m=1}^{M} v_{2m} r^{2m} \tag{4.7}$$

and, hence, the eigenvalues of the original equation can be examined by the radial Schrödinger equation in (4.1). As we pointed out earlier, potentials (3.3) and (3.5) are

Table 11. Convergence rates of eigenvalue bounds as a function of ℓ, for the ground-state energy of the sextic oscillator in (4.6), which is determined analytically, i.e. $E_{0,0,0} = 6$, in the unbounded domain.

ℓ	N	$E^-_{0,0,0}(\ell)$	$E^+_{0,0,0}(\ell)$
1.00	5	3.3	8.4
1.50	5	5.933	6.051
1.75	5	5.9980	6.0017
2.00	7	5.999 986	6.000 014
2.25	9	5.999 999 982	6.000 000 018
2.30	10	5.999 999 996	6.000 000 004
2.35	11	5.999 999 9993	6.000 000 0007
2.40	11	5.999 999 999 88	6.000 000 000 12
2.45	12	5.999 999 999 982	6.000 000 000 018
2.50	13	5.999 999 999 9974	6.000 000 000 0025

examples of this case when $\alpha = 1$ and $\beta = \gamma = 1$, respectively. It can be deduced that our bounds in tables 3–5 with $\alpha = 1$ are very good and consistent with the results of the isotropic quartic oscillator already available in the literature [20–22]. Note that the notation of the authors of [20, 21] differ from that of the present paper so that their anharmonicity constants and eigenvalues should either be divided or multiplied by 2, or *vice versa*. We have not introduced, however, any numerical table for a particular comparison in order not to overfill the content of the paper with tabular material. Moreover, the eigensolutions of the sextic oscillators $V(r) = v_2r^2 + v_4r^4 + v_6r^6$ can be derived analytically for special values of the parameters, similar to those of the one-dimensional case. The confidence in the accuracy of our two-sided bounds has also been reconfirmed by utilizing exact results so determined.

In conclusion, the accurate results presented in the tables provide a rich information about the spectral properties, which may be regarded as a guide to future numerical methods to be developed for solving three-dimensional eigenvalue problems of this kind. It is worth noting that the applicability of our method is not limited by the examples which are numerically studied here. In contrast, the algorithm is sufficiently general in its structure to incorporate any physical, more interesting, potentials having convergent power series expansions about the origin. This follows from the fact that such potentials can approximately be characterized by the arbitrary polynomial in (1.2), for which the method is established. Note also that we are interested only in the energetic structure of the Schrödinger Hamiltonians calculating the spectral points. The eigenfunctions may be examined as well to shed some light on the global behaviour of the system. For instance, we have perceived, from table 1, that the rate of convergence of the successive approximations, as N and ℓ increase, is relatively slow for the eigenvalues of the potential (1.3), which is perhaps an example of a chaotic system. Now that we are encouraged by the success of the confined system approximation, more interesting problems such as chaotic Hamiltonians will be investigated in the near future.

Acknowledgments

The authors are grateful to the referees for making valuable comments and suggestions for the improvement of the paper. The discussion in the last three paragraphs follows suggestions by the referees.

Appendix. Variation of eigenvalues with respect to the confinement parameter in the Dirichlet and Neumann problems

It is obvious that the eigensolutions of the enclosed Schrödinger equation (1.1), in which $\mathbb{R}^3$ is replaced by Ω, depend on the boundary parameter ℓ. Therefore, any normalized eigenfunction and the corresponding eigenvalue may be denoted by

$$\Psi = \Psi(x, y, z; \ell) \tag{A.1}$$

and

$$E = E(\ell) \tag{A.2}$$

respectively. Now, we present a theoretical analysis on the behaviour of $E(\ell)$ when the wavefunction satisfies the Dirichlet and Neumann boundary conditions. Rewriting equation (1.1) in the form

$$\mathcal{L}\Psi = 0 \qquad \mathcal{L} = -\nabla^2 + V(x, y, z) - E(\ell) \tag{A.3}$$

on differentiating both sides with respect to ℓ, we obtain

$$\Psi \frac{\mathrm{d}E}{\mathrm{d}\ell} = \mathcal{L}\Psi_\ell. \tag{A.4}$$

If we multiply (A.4) by Ψ and integrate over the three-dimensional space Ω, it follows immediately that

$$\frac{\mathrm{d}E}{\mathrm{d}\ell} = \langle \mathcal{L}\Psi_\ell, \Psi \rangle \tag{A.5}$$

where ket and bra notation stands for the inner product. Introducing the formal adjoint of the operator $\mathcal{L}$, we then find that

$$\frac{\mathrm{d}E}{\mathrm{d}\ell} = \text{surface integral terms} + \langle \Psi_\ell, \mathcal{L}^\star \Psi \rangle \tag{A.6}$$

in which the inner product on the right-hand side vanishes from (A.3) since $\mathcal{L}$ is formally self-adjoint with $\mathcal{L}^\star = \mathcal{L}$. Thus we have

$$\frac{\mathrm{d}E}{\mathrm{d}\ell} = \int_{-\ell}^{\ell}\int_{-\ell}^{\ell} (\Psi_x \Psi_\ell - \Psi \Psi_{x\ell})|_{x=-\ell}^{\ell}\, \mathrm{d}y\, \mathrm{d}z + \int_{-\ell}^{\ell}\int_{-\ell}^{\ell} (\Psi_y \Psi_\ell - \Psi \Psi_{y\ell})|_{y=-\ell}^{\ell}\, \mathrm{d}x\, \mathrm{d}z$$
$$+ \int_{-\ell}^{\ell}\int_{-\ell}^{\ell} (\Psi_z \Psi_\ell - \Psi \Psi_{z\ell})|_{z=-\ell}^{\ell}\, \mathrm{d}x\, \mathrm{d}y \tag{A.7}$$

which may be simplified by using the boundary conditions.

In order to understand the meaning of partial derivatives with respect to ℓ, let us first consider the total differential of $\Psi(x, y, z; \ell)$,

$$\mathrm{d}\Psi = \Psi_x\, \mathrm{d}x + \Psi_y\, \mathrm{d}y + \Psi_z\, \mathrm{d}z + \Psi_\ell\, \mathrm{d}\ell. \tag{A.8}$$

Nevertheless if, for instance, x is a function of ℓ, $x = f(\ell)$, then $\mathrm{d}x = (\mathrm{d}f/\mathrm{d}\ell)\,\mathrm{d}\ell$ and hence

$$\mathrm{d}\Psi = \Psi_y\, \mathrm{d}y + \Psi_z\, \mathrm{d}z + \left(\Psi_\ell + \frac{\mathrm{d}f}{\mathrm{d}\ell}\Psi_x\right)\mathrm{d}\ell \tag{A.9}$$

implying the operational equivalence

$$\Psi_\ell = \Psi_\ell + \frac{\mathrm{d}f}{\mathrm{d}\ell}\Psi_x. \tag{A.10}$$

Here, Ψ_ℓ on the left-hand side should be regarded as the partial derivative of the function $\Psi[f(\ell), y, z; \ell]$ of ℓ, y and z only. So

$$\Psi_\ell = \Psi_\ell \mp \Psi_x \tag{A.11}$$

when $x = f(\ell) = \mp\ell$. Likewise, we see that

$$\Psi_\ell = \Psi_\ell \mp \Psi_y \qquad \text{and} \qquad \Psi_\ell = \Psi_\ell \mp \Psi_z \tag{A.12}$$

when $y = \mp\ell$ and $z = \mp\ell$, respectively. In accordance with (A.11) and (A.12), the partial differentiation with respect to ℓ of the Dirichlet conditions in (1.7) and the Neumann conditions in (1.8) lead to the equations

$$\begin{aligned}
&\Psi_\ell(\mp\ell, y, z) \mp \Psi_x(\mp\ell, y, z) = 0\\
&\Psi_\ell(x, \mp\ell, z) \mp \Psi_y(x, \mp\ell, z) = 0\\
&\Psi_\ell(x, y, \mp\ell) \mp \Psi_z(x, y, \mp\ell) = 0
\end{aligned} \tag{A.13}$$

and

$$\begin{aligned}
&\Psi_{x\ell}(\mp\ell, y, z) \mp \Psi_{xx}(\mp\ell, y, z) = 0\\
&\Psi_{y\ell}(x, \mp\ell, z) \mp \Psi_{yy}(x, \mp\ell, z) = 0\\
&\Psi_{z\ell}(x, y, \mp\ell) \mp \Psi_{zz}(x, y, \mp\ell) = 0
\end{aligned} \tag{A.14}$$

respectively. Therefore, in the case of the Dirichlet problem, substitution of Ψ_ℓ from (A.14) into (A.7) gives

$$\begin{aligned}
\frac{\mathrm{d}E^+}{\mathrm{d}\ell} = &-\int_{-\ell}^{\ell}\int_{-\ell}^{\ell}[\Psi_x^2(\ell, y, z) + \Psi_x^2(-\ell, y, z)]\,\mathrm{d}y\,\mathrm{d}z\\
&-\int_{-\ell}^{\ell}\int_{-\ell}^{\ell}[\Psi_y^2(x, \ell, z) + \Psi_y^2(x, -\ell, z)]\,\mathrm{d}x\,\mathrm{d}z\\
&-\int_{-\ell}^{\ell}\int_{-\ell}^{\ell}[\Psi_z^2(x, y, \ell) + \Psi_z^2(x, y, -\ell)]\,\mathrm{d}x\,\mathrm{d}y
\end{aligned} \tag{A.15}$$

from which (1.9) is obtained by exploiting the reflection symmetries of the wavefunction. In any case, however, we have shown that

$$\frac{\mathrm{d}E^+}{\mathrm{d}\ell} < 0 \tag{A.16}$$

which completes the proof on the decreasing behaviour of $E^+(\ell)$.

If we use the Neumann conditions (1.8) and the relations in (A.15), equation (A.7) takes the form

$$\begin{aligned}
\frac{\mathrm{d}E^-}{\mathrm{d}\ell} = &\int_{-\ell}^{\ell}\int_{-\ell}^{\ell}[\Psi(\ell, y, z)\Psi_{xx}(\ell, y, z) + \Psi(-\ell, y, z)\Psi_{xx}(-\ell, y, z)]\,\mathrm{d}y\,\mathrm{d}z\\
&+\int_{-\ell}^{\ell}\int_{-\ell}^{\ell}[\Psi(x, \ell, z)\Psi_{yy}(x, \ell, z) + \Psi(x, -\ell, z)\Psi_{yy}(x, -\ell, z)]\,\mathrm{d}x\,\mathrm{d}z\\
&+\int_{-\ell}^{\ell}\int_{-\ell}^{\ell}[\Psi(x, y, \ell)\Psi_{zz}(x, y, \ell) + \Psi(x, y, -\ell)\Psi_{zz}(x, y, -\ell)]\,\mathrm{d}x\,\mathrm{d}y.
\end{aligned} \tag{A.17}$$

Furthermore, examining the first integral

$$I_1 = \int_{-\ell}^{\ell}\int_{-\ell}^{\ell} \Psi(\ell, y, z)\Psi_{xx}(\ell, y, z)\,\mathrm{d}y\,\mathrm{d}z \tag{A.18}$$

in (A.17) we may derive a more useful expression for $\mathrm{d}E^-/\mathrm{d}\ell$. Indeed, from (A.3), I_1 can be put in the form

$$I_1 = \int_{-\ell}^{\ell}\int_{-\ell}^{\ell}[V(\ell, y, z) - E^-]\Psi^2(\ell, y, z)\,\mathrm{d}y\,\mathrm{d}z - \int_{-\ell}^{\ell}\int_{-\ell}^{\ell}\Psi(\ell, y, z)[\Psi_{yy}(\ell, y, z) + \Psi_{zz}(\ell, y, z)]\,\mathrm{d}y\,\mathrm{d}z \tag{A.19}$$

for which the last term is integrated by parts to obtain

$$I_1 = \int_{-\ell}^{\ell}\int_{-\ell}^{\ell}\left\{[V(\ell, y, z) - E^-]\Psi^2(\ell, y, z) + \Psi_y^2(\ell, y, z) + \Psi_z^2(\ell, y, z)\right\}\mathrm{d}y\,\mathrm{d}z. \tag{A.20}$$

Other integrals are evaluated by repeating the same process, and, therefore, equation (A.17) becomes

$$\begin{aligned}\frac{\mathrm{d}E^-}{\mathrm{d}\ell} = &\int_{-\ell}^{\ell}\int_{-\ell}^{\ell}\{[V(\ell, y, z) - E^-]\Psi^2(\ell, y, z) + \Psi_y^2(\ell, y, z) + \Psi_z^2(\ell, y, z)\\ &+[V(-\ell, y, z) - E^-]\Psi^2(-\ell, y, z) + \Psi_y^2(-\ell, y, z) + \Psi_z^2(-\ell, y, z)\}\,\mathrm{d}y\,\mathrm{d}z\\ &+\int_{-\ell}^{\ell}\int_{-\ell}^{\ell}\{[V(x, \ell, z) - E^-]\Psi^2(x, \ell, z) + \Psi_x^2(x, \ell, z) + \Psi_z^2(x, \ell, z)\\ &+[V(x, -\ell, z) - E^-]\Psi^2(x, -\ell, z) + \Psi_x^2(x, -\ell, z) + \Psi_z^2(x, -\ell, z)\}\,\mathrm{d}x\,\mathrm{d}z\\ &+\int_{-\ell}^{\ell}\int_{-\ell}^{\ell}\{[V(x, y, \ell) - E^-]\Psi^2(x, y, \ell) + \Psi_x^2(x, y, \ell) + \Psi_y^2(x, y, \ell)\\ &+[V(x, y, -\ell) - E^-]\Psi^2(x, y, -\ell) + \Psi_x^2(x, y, -\ell) + \Psi_y^2(x, y, -\ell)\}\,\mathrm{d}x\,\mathrm{d}y.\end{aligned} \tag{A.21}$$

Under the assumption that the wavefunction possesses the reflection symmetries, this equation reduces to the form of (1.10). Consequently,

$$\frac{\mathrm{d}E^-}{\mathrm{d}\ell} > 0 \tag{A.22}$$

subject to the sufficient condition that $|\ell|$ is beyond the classical turning points.

References

[1] Hioe F T, MacMillen D and Montroll E W 1976 *J. Math. Phys.* **17** 1320
[2] Banerjee K 1978 *Prog. R. Soc. Lond.* A **364** 265
[3] Blankenbecler R, DeGrant T and Sugar R L 1980 *Phys. Rev.* D **21** 1055
[4] Killingbeck J, Jones M N and Thompson M J 1985 *J. Phys. A: Math. Gen.* **18** 793
[5] Taşeli H and Demiralp M 1988 *J. Phys. A: Math. Gen.* **21** 3903
[6] Handy C R 1995 *Phys. Rev.* A **52** 3468
[7] Vrscay E R and Handy C R 1989 *J. Phys. A: Math. Gen.* **22** 823
[8] Banks T, Bender C M and Wu T T 1973 *Phys. Rev.* D **8** 3346
[9] Hioe F T, MacMillen D and Montroll E W 1978 *Phys. Rep.* **43** 305
[10] Ari N and Demiralp M 1985 *J. Math. Phys.* **26** 1179
[11] Fernandez F M, Meson A M and Castro E A 1985 *Phys. Lett.* **112A** 107
[12] Witwit M R M 1992 *J. Math. Phys.* **33** 4196
[13] Bender C M and Wu T T 1969 *Phys. Rev.* **184** 1231
[14] Witwit M R M 1992 *J. Math. Phys.* **33** 2779
[15] Taşeli H 1992 *J. Comput. Phys.* **101** 252
[16] Taşeli H and Eid R 1996 *Int. J. Quantum Chem.* **59** 183
[17] Taşeli H 1996 *Int. J. Quantum Chem.* **60** 641

[18] Taşeli H and Eid R 1996 *J. Phys. A: Math. Gen.* **29** 6967
[19] Taşeli H and Zafer A 1997 *Int. J. Quantum Chem.* **61** 759
[20] Seetharaman M and Vasan S S 1986 *J. Math. Phys.* **27** 1031
[21] Lakshmanan M, Kaliappan P, Larsson K, Karlsson F and Fröman P O 1994 *Phys. Rev.* A **49** 3296
[22] Taşeli H 1996 *J. Math. Chem.* **20** 235