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An eigenfunction expansion for the Schrödinger equation with arbitrary non-central potentials

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An eigenfunction expansion for the Schrödinger equation for a particle moving in an arbitrary non-central potential in the cylindrical polar coordinates is introduced, which reduces the partial differential equation to a system of coupled differential equations in the radial variable r. It is proved that such an orthogonal expansion of the wavefunction into the complete set of Chebyshev polynomials is uniformly convergent on any domain of (r, θ). As a benchmark application, the bound states calculations of the quartic oscillator show that both analytical and numerical implementations of the present method are quite satisfactory.

KEY WORDS: two-dimensional Schrödinger equation, eigenfunction expansion, eigenvalue problems

1. Introduction

A mathematical problem in applied sciences generally consists of dealing with differential equations of certain type which govern the behaviours of certain physical, or other, quantities. Probably the most frequently occuring equation of this type in quantum mechanics is the stationary Schrödinger equation for the wavefunction. The probability densities and the total energies of a quantum system are determined by means of the solutions (i.e. eigenvalues and eigenfunctions) of such an eigenvalue problem in which the admissible wavefunction also satisfies prescribed conditions on the surfaces bounding the region being considered. Unfortunately, however, the analytic solvability of the Schrödinger equation even in one dimension is restricted to a few classes of potentials. Therefore, the use of approximation methods for the relevant computational problem gains a lot of significance. In spite of the development of many reliable methods and techniques for the one-dimensional case by the advent of powerful computers, the treatment of the problem in more than one dimension is still a non-trivial task. In general, the applicability of well established methods such as perturbative, variational, etc. [1–6], is not as practical as in the one dimension. Clearly, the multi-dimensional Schrödinger equation for a spherically symmetric potential may be regarded as one-dimensional since it is described by an ordinary differential equation (ODE) in the single variable of the hyper-radial coordinate r.

On the other hand, solutions of a linear partial differential equation (PDE) are often expressible as *Generalized Fourier Series* if we have a suitable expansion basis at hand. Such a formal solution can also be called an *eigenfunction expansion* because the set of basis functions is, in general, a complete set of eigenfunctions of a Sturm–Liouville system. An eigenfunction expansion of this kind reduces the PDE to a system of ODEs, which contains coupled ODEs whenever the original PDE is non-separable. In particular, the three-dimensional Schrödinger equation with a specific non-central potential in the spherical polar coordinates (r, θ, ϕ) can be converted into a system of ODEs by expanding the wavefunction in terms of spherical harmonics [7]. However, the analysis in [7] includes those specific potentials for which the Schrödinger equation is separable, and, hence, leads to uncoupled ODEs. In fact, the study of the Schrödinger equation with an arbitrary potential by means of an eigenfunction expansion has received less attention and even never appeared in the literature in the two-dimensional case.

In this article we, therefore, focus our attention to the Schrödinger PDE written in the two-dimensional cylindrical polar coordinates (r, θ). It is shown in section 2 that the wavefunction has a convergent series expansion in terms of the Chebyshev polynomials. The reduction of the PDE to a coupled system of ODEs is introduced in section 3 with the related technicalities. Our approach is applied to the well known quartic oscillator in section 4 to analyze the numerical performance of the resulting computational problem. The concluding remarks and comments are made in the last section.

2. Eigenfunction expansion

The Schrödinger equation for a particle in the presence of a scalar potential $V(r, \theta)$ is written as

$$\left[-\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right)-\frac{1}{r^2}\frac{\partial^2}{\partial\theta^2}+V(r,\theta)\right]\Psi = E\Psi, \qquad r \in [0,\infty), \quad \theta \in [-\pi,\pi], \tag{2.1}$$

in the cylindrical polar coordinates. We assume that the real wavefunction $\Psi(r, \theta)$ belongs to the Hilbert space of the square integrable functions, i.e.

$$\langle \Psi, \Psi \rangle < \infty, \tag{2.2}$$

where

$$\langle f, g \rangle = \int_{-\pi}^{\pi}\int_0^{\infty} f(r,\theta)g(r,\theta)r \,\mathrm{d}r\,\mathrm{d}\theta, \tag{2.3}$$

and the potential function $V(r, \theta)$ is either an even or an odd function of θ. Furthermore, it does not grow faster than r^{-1} as $r \to 0$, and $rV(r, \theta)$ has no singularity on any subregion of the region under consideration. If we make the substitution

$$\eta = \cos\theta, \quad \eta \in [-1, 1], \tag{2.4}$$

the PDE and the square integrability condition are transformed into

$$\left\{-\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right)-\frac{1}{r^2}\left[\left(1-\eta^2\right)\frac{\partial^2}{\partial \eta^2}-\eta\frac{\partial}{\partial \eta}\right]+V(r,\eta)\right\}\Psi=E\Psi \qquad (2.5)$$

and

$$2\int_{-1}^{1}\int_{0}^{\infty}\left[\Psi(r,\eta)\right]^2\left(1-\eta^2\right)^{-1/2} r\,\mathrm{d}r\,\mathrm{d}\eta<\infty, \qquad (2.6)$$

respectively. The restriction on $V(r,\theta)$ of being an even or odd function of θ follows from the fact that the mapping in (2.4) is not one-to-one. In fact, many potentials encountered in practice fall into this catagory.

It is obvious that the η-dependence of (2.5) is closely related to the differential operator in the eigenvalue problem which generates the orthogonal sequence of Chebyshev polynomials of the first kind $T_n(\eta)$ over the interval $\eta \in [-1,1]$. Moreover, the square integrability condition in (2.6) suggests that the following integral is also bounded:

$$\int_{-1}^{1}\left[\Psi(r,\eta)\right]^2\left(1-\eta^2\right)^{-1/2}\,\mathrm{d}\eta<\infty \qquad (2.7)$$

for any fixed r, $r \in \mathbb{R}^+$, where $\mathbb{R}^+$ stands for the set of real positive numbers. Thus, for each $r \in \mathbb{R}^+$, the sequence of functions

$$\Phi_n(r,\eta)=\sum_{k=0}^{n} R_k(r)T_k(\eta), \quad n=0,1,\ldots, \qquad (2.8)$$

converges in the mean as $n \to \infty$ to the exact solution $\Psi(r,\eta)$ of the problem (2.5) and (2.6), provided that the $R_k(r)$ are the so-called Fourier coefficients. That is, if

$$\|f\|^2=\int_{-1}^{1}\left[f(\eta)\right]^2\left(1-\eta^2\right)^{-1/2}\,\mathrm{d}\eta \qquad (2.9)$$

denotes the norm of a function of $\eta \in [-1,1]$, then

$$\lim_{n\to\infty}\left\|\Psi(r,\eta)-\Phi_n(r,\eta)\right\|=0 \qquad (2.10)$$

for each $r \in \mathbb{R}^+$. It is known that the Fourier coefficients are defined by

$$R_k(r)=\mathcal{N}_k^{-1}\int_{-1}^{1}\Psi(r,\eta)T_k(\eta)\left(1-\eta^2\right)^{-1/2}\,\mathrm{d}\eta, \qquad (2.11)$$

where

$$\mathcal{N}_k=\begin{cases}\pi & \text{for } k=0,\\ \pi/2 & \text{for } k>0,\end{cases} \qquad (2.12)$$

is the orthonormalization constant for the Chebyshev polynomials.

The expansion in (2.8) is valid only in the case of a potential $V(r,\theta)$ which is an even function of θ. If $V(r,\theta)$ is an odd function of θ then the expansion basis $\{T_n(\eta)\}$

with $n = 0, 1, \ldots$ should be replaced by $\{\sqrt{1-\eta^2}U_{n-1}(\eta)\}$ with $n = 1, 2, \ldots,$ where the $\{U_{n-1}(\eta)\}$ are the Chebyshev polynomials of the second kind. Note that the functions $T_n(\eta)$ and $\sqrt{1-\eta^2}U_{n-1}(\eta)$ satisfy the same differential equation as well as the same functional relationships, so that our analysis remains unaltered in form. Note also that for a potential which is neither even nor odd in θ, it would have been much more straightforward to stay with the original equation (2.1) and to represent the wavefunction as a series expansion in terms of the sequence of complex exponentials $\{\mathrm{e}^{\mathrm{i}n\theta}\}$ for $n = 0, \mp 1, \mp 2, \ldots.$ Therefore, the even or odd structure of the potential in θ variable makes it possible to split the set $\{\mathrm{e}^{\mathrm{i}n\theta}\}$ into two subsets containing even and odd functions of θ separately. Then the transformation in (2.4) allows dealing with the Chebyshev polynomials rather than the trigonometric functions in a more systematic way.

The square integrability condition for the wavefunction in (2.7) implies merely that, for a fixed r, Ψ is Lebesgue measurable on $-1 \leqslant \eta \leqslant 1$, i.e. $\Psi \in \mathcal{L}^2(-1, 1)$. As a result, we have stated in (2.10) that the limit of the set of functions $\{\Phi_n\}$ converges to the wavefunction in the norm (2.9) of $\mathcal{L}^2(-1, 1)$. In fact, it can be shown that $\{\Phi_n(r, \eta)\}$ converges uniformly to $\Psi(r, \eta)$ on $\eta \in [-1, 1]$ for every positive r.

Proposition 1. Let $r \in \mathbb{R}^+$ be a fixed number. Then the expansion of the wavefunction in terms of the Chebyshev polynomials

$$\lim_{n\to\infty} \Phi_n(r, \eta) = \sum_{k=0}^{\infty} R_k(r) T_k(\eta) \tag{2.13}$$

converges uniformly to $\Psi(r, \eta)$ for all $\eta \in [-1, 1]$.

Proof. From (2.11), we write

$$R_0(r) = \mathcal{N}_0^{-1} \int_{-1}^{1} \Psi(r, \eta)\left(1-\eta^2\right)^{-1/2} \mathrm{d}\eta \tag{2.14}$$

in which we have used the identity $T_0(\eta) = 1$. By the mean value theorem for integrals we have

$$R_0(r) = \mathcal{N}_0^{-1}\Psi(r, \eta_0) \int_{-1}^{1} \left(1-\eta^2\right)^{-1/2} \mathrm{d}\eta = \Psi(r, \eta_0), \tag{2.15}$$

where η_0 is some constant on $-1 \leqslant \eta \leqslant 1$. So $R_0(r)$ is absolutely bounded by $\rho_0(r)$,

$$\left|R_0(r)\right| \leqslant \rho_0(r), \quad \rho_0(r) = \max_{\eta\in[-1,1]} \left|\Psi(r, \eta)\right|. \tag{2.16}$$

For $k = 1, 2, \ldots,$ using the relation $T_k(\eta) = \cos(k \arccos \eta)$ and integrating (2.11) by parts twice, we get

$$R_k(r) = \mathcal{N}_k^{-1} k^{-2} \int_{-1}^{1} \left[\eta \frac{\partial \Psi}{\partial \eta} - \left(1-\eta^2\right) \frac{\partial^2 \Psi}{\partial \eta^2}\right] \left(1-\eta^2\right)^{-1/2} \mathrm{d}\eta \tag{2.17}$$

which yields

$$\left|R_k(r)\right| \leqslant \frac{2\rho(r)}{k^2}, \tag{2.18}$$

where

$$\rho(r) = \max_{\eta\in[-1,1]} \left|\eta\frac{\partial\Psi}{\partial\eta} - \left(1-\eta^2\right)\frac{\partial^2\Psi}{\partial\eta^2}\right|. \tag{2.19}$$

The functional series in (2.13) satisfies the obvious inequalities

$$\sum_{k=0}^{\infty} R_k(r)T_k(\eta) \leqslant \sum_{k=0}^{\infty} \left|R_k(r)\right|\left|T_k(\eta)\right| \leqslant \sum_{k=0}^{\infty} \left|R_k(r)\right| \tag{2.20}$$

since $|T_k(\eta)| \leqslant 1$. Furthermore, taking (2.16) and (2.18) into account, we now derive

$$\sum_{k=0}^{\infty} \left|R_k(r)\right| \leqslant \rho_0(r) + 2\rho(r)\sum_{k=1}^{\infty} k^{-2} = \rho_0(r) + 2\rho(r)\zeta(2), \tag{2.21}$$

where $\zeta(2) = \pi^2/6$ is a well-known special value of the Riemann zeta function $\zeta(n) = \sum_{k=1}^{\infty} k^{-n}$ for $n = 2, 3, \ldots$ [8]. According to the Weierstrass test, it follows that our series converges uniformly as it can be majorized by a convergent series

$$\sum_{k=0}^{\infty} R_k(r)T_k(\eta) \leqslant \rho_0(r) + \frac{\pi^2\rho(r)}{3}. \tag{2.22}$$

More precisely, there exists a function, $\Phi(r,\eta)$ say, to which $\Phi_n(r,\eta)$ converges uniformly as $n \to \infty$ on the set $\eta \in [-1,1]$ for a fixed $r \in \mathbb{R}^+$. Since the fixed value of r is any representative number, we can conclude that the proposition holds for all r saving the points at the origin and infinity. Note also that such positive r's are all ordinary points of the PDE so that $\rho_0(r)$ and $\rho(r)$ depending on the actual solution Ψ denote continuous and, hence, bounded functions.

It remains now to show that the function $\Phi(r,\eta)$ is nothing but a representation of the wavefunction $\Psi(r,\eta)$. Clearly, the uniform convergence of Φ_n implies that

$$0 \leqslant \|\Phi_n - \Phi\| = \left\{\int_{-1}^{1} \left[\Phi_n(r,\eta) - \Phi(r,\eta)\right]^2 \left(1-\eta^2\right)^{-1/2} \mathrm{d}\eta\right\}^{1/2} \leqslant \frac{\varepsilon_n}{2}, \tag{2.23}$$

where

$$\varepsilon_n = 2\max_{\eta\in[-1,1]} \left|\Phi_n(r,\eta) - \Phi(r,\eta)\right|\sqrt{\pi}, \tag{2.24}$$

and that Φ_n converges to Φ in the sense of $\mathcal{L}^2(-1,1)$ norm as well, for large enough values of n. From (2.10) and the triangle inequality, we have the relations

$$0 \leqslant \|\Psi - \Phi\| \leqslant \|\Psi - \Phi_n\| + \|\Phi_n - \Phi\| \leqslant \frac{\varepsilon_n}{2} + \frac{\varepsilon_n}{2} = \varepsilon_n \tag{2.25}$$

leading to

$$\|\Psi - \Phi\|^2 = \int_{-1}^{1} \big[\Psi(r,\eta) - \Phi(r,\eta)\big]^2 \big(1-\eta^2\big)^{-1/2}\,\mathrm{d}\eta = 0 \tag{2.26}$$

in the limiting case as $n \to \infty$. It follows then that

$$\Psi(r,\eta) = \Phi(r,\eta) = \sum_{k=0}^{\infty} R_k(r) T_k(\eta) \tag{2.27}$$

for all $\eta \in [-1, 1]$ and $r \in \mathbb{R}^+$. This completes the proof. □

The formal series for Ψ will be the required solution if it really satisfies the square integrability condition (2.6). The asymptotic forms of Ψ at the boundaries of r-interval, $r = 0$ and $r \to \infty$, are of considerable importance to this end [9]. It is shown that the singular points of the PDE are located at $r = 0$ and $r \to \infty$, the former being a regular singularity. Therefore, the proper solution should remain finite at the origin and should have an appropriate vanishing behaviour at infinity.

Proposition 2. If the $R_k(r)$ behave like r^k, $R_k(r) = \mathrm{O}(r^k)$, as $r \to 0$, then the series in (2.27) remains finite at the origin.

Proof. For sufficiently small values of r, (2.27) can be written as

$$\Psi(r,\eta) \sim c \sum_{k=0}^{\infty} r^k T_k(\eta), \tag{2.28}$$

where the constant c has been assumed to be the maximum of the parameters c_k in the relation $|R_k(r)| \leqslant c_k |r^k|$. Recalling the generating function of the Chebyshev polynomials [8], it follows that

$$\Psi(r,\eta) \sim \frac{1}{2} c \left(\frac{1-r^2}{1-2\eta r + r^2} + 1 \right) \tag{2.29}$$

as $r \to 0$, which yields the finite value of c at $r = 0$ for all η. □

Proposition 3. If the functions $R_k(r)$ decay exponentially at infinity, that is, $R_k(r) = \mathrm{O}(\mathrm{e}^{-ar^b})$ as $r \to \infty$ for some positive a and b parameters independent of k, so does $\Psi(r,\eta)$.

Proof. Using the fact that $|T_k(\eta)| \leqslant 1$ we introduce the two-sided inequalities

$$-(n+1) \leqslant \sum_{k=0}^{n} T_k(\eta) \leqslant n+1 \tag{2.30}$$

for the sum of the first $n+1$ Chebyshev polynomials, which lead to the relations

$$-(n+1)\,\mathrm{e}^{-ar^b} \leqslant \sum_{k=0}^{n} \mathrm{e}^{-ar^b} T_k(\eta) \leqslant (n+1)\,\mathrm{e}^{-ar^b}. \tag{2.31}$$

When n and r are both sufficiently large of the same order or $n \sim r^m$ with $m \in \mathbb{R}$, equation (2.31) is equivalent to

$$-\left(r^m+1\right)\mathrm{e}^{-ar^b} \leqslant \Phi_n(r,\eta) \leqslant \left(r^m+1\right)\mathrm{e}^{-ar^b}. \tag{2.32}$$

Hence, passing to the limit we see that

$$0 \leqslant \lim_{r,n\to\infty} \Phi_n(r,\eta) \leqslant 0 \tag{2.33}$$

and that

$$\lim_{r\to\infty} \Psi(r,\eta) = 0. \tag{2.34}$$

So, the series expansion for Ψ vanishes exponentially at infinity, which completes the proof. □

Corollary. The series representation of the wavefunction in (2.27) satisfies the square integrability condition.

Proof. If we substitute (2.27) into (2.6), interchange formally one summation and the integral operation with respect to η and, thus, use the orthogonality of the Chebyshev polynomials once more, the square integrability condition takes the form

$$2\int_{-1}^{1}\int_{0}^{\infty} \left[\Psi(r,\eta)\right]^2 \left(1-\eta^2\right)^{-1/2} r\,\mathrm{d}r\,\mathrm{d}\eta = 2\int_0^\infty \sum_{k=0}^{\infty} \mathcal{N}_k\left[R_k(r)\right]^2 r\,\mathrm{d}r < \infty. \tag{2.35}$$

Therefore, we should have

$$\pi\int_0^\infty \left[\sigma(r)\right]^2 \mathrm{d}r < \infty, \tag{2.36}$$

where

$$\sigma(r) = \left\{\left[\sqrt{2r}\,R_0(r)\right]^2 + \sum_{k=1}^{\infty}\left[\sqrt{r}\,R_k(r)\right]^2\right\}^{1/2}. \tag{2.37}$$

It is readily seen, from (2.16) and (2.18), that the integrand is dominated by

$$\left[\sigma(r)\right]^2 \leqslant 2r\left[\rho_0(r)\right]^2 + 4r\left[\rho(r)\right]^2 \sum_{k=1}^{\infty} k^{-4} = 2r\left\{\left[\rho_0(r)\right]^2 + 2\zeta(4)\left[\rho(r)\right]^2\right\} \tag{2.38}$$

in which the functions $\rho_0(r)$ and $\rho(r)$ depend solely on the exact wavefunction Ψ, as shown in proposition 1. On the other hand, the proposed series expansion of Ψ behaves correctly at the end points of the range of r by propositions 2 and 3, verifying *a posteriori* the existence of the improper integral in (2.36). $\square$

Further comments on the function $\sigma(r)$ will be included in the next section.

3. The system of coupled ODEs

We have asserted the expansion of the wavefuntion into the complete set of Chebyshev polynomials. As a result, the substitution of Ψ in (2.27) into the Schrödinger equation (2.5) and the elimination of the partial derivatives with respect to η from the ODE for the Chebyshev polynomials [8], it follows that

$$\sum_{k=0}^{\infty}\left[-\frac{1}{r}\frac{\mathrm{d}}{\mathrm{d}r}\left(r\frac{\mathrm{d}}{\mathrm{d}r}\right)+\frac{k^2}{r^2}+V(r,\eta)-E\right]R_k(r)T_k(\eta)=0. \tag{3.1}$$

The expansion of the product $V(r,\eta)T_k(\eta)$ into a series of the $T_j(\eta)$,

$$V(r,\eta)T_k(\eta)=\sum_{j=0}^{\infty}f_{kj}(r)T_j(\eta), \tag{3.2}$$

can be justified by the assumptions in section 2 on the potential function $V(r,\eta)$. Here a matrix $\mathbf{f}\triangleq[f_{jk}]$ whose general entry is defined by

$$f_{jk}(r)=\mathcal{N}_k^{-1}\int_{-1}^{1}V(r,\eta)T_j(\eta)T_k(\eta)\left(1-\eta^2\right)^{-1/2}\mathrm{d}\eta,\quad j,k=0,1,\ldots, \tag{3.3}$$

may be regarded as a matrix representation of $V(r,\eta)T_k(\eta)$. We see that the f_{jk} have the properties

$$f_{j0}=\frac{1}{2}f_{0j},\quad f_{jk}=f_{kj},\qquad j,k=1,2,\ldots \tag{3.4}$$

between the two indexes. Now transforming the dependent variable from $R_k(r)$ to $\mathcal{R}_k(r)$, for convenience, where

$$\mathcal{R}_k(r)=r^{1/2}R_k(r),\quad k=0,1,\ldots, \tag{3.5}$$

and employing (3.2) and the fact that the $T_k(\eta)$ are linearly independent, we obtain from (3.1) the coupled system of ODEs

$$\sum_{k=0}^{\infty}(H_{jk}-E\delta_{jk})\mathcal{R}_k(r)=0,\quad j=0,1,\ldots, \tag{3.6}$$

for the determination of the functions $\mathcal{R}_k(r)$. Here, $\mathbf{H}\triangleq[H_{jk}]$ is a matrix-differential operator of the form

$$H_{jk}=\left[-\frac{\mathrm{d}^2}{\mathrm{d}r^2}+\left(k^2-\frac{1}{4}\right)\frac{1}{r^2}\right]\delta_{jk}+f_{jk},\quad j,k=0,1,\ldots, \tag{3.7}$$

and δ_{jk} stands for the Kronecker delta.

If the $\mathcal{R}_k(r)$ are identified as the components of a vector-valued function, $\boldsymbol{\mathcal{R}}(r)$ say,

$$\boldsymbol{\mathcal{R}}(r) \triangleq [\mathcal{R}_0(r), \mathcal{R}_1(r), \ldots, \mathcal{R}_k(r), \ldots]^{\mathrm{T}}, \tag{3.8}$$

then the system in (3.6) refers to the infinite-dimensional vector differential equation

$$(\mathbf{H} - E\mathbf{I})\boldsymbol{\mathcal{R}}(r) = \mathbf{0}, \quad r \in [0, \infty), \tag{3.9}$$

where $\mathbf{I} \triangleq [\delta_{jk}]$ is the identity matrix.

The conditions accompanying with the vector differential equation can easily be deduced from propositions 2 and 3 of section 2. Furthermore, the function $\sigma(r)$ in (2.37) is very closely related to the norm of the vector $\boldsymbol{\mathcal{R}}(r)$

$$\left\|\boldsymbol{\mathcal{R}}(r)\right\|^2 = \boldsymbol{\mathcal{R}}^{\mathrm{T}}(r) \cdot \boldsymbol{\mathcal{R}}(r) = \sum_{k=0}^{\infty} \left[\mathcal{R}_k(r)\right]^2 = \left[\sigma(r)\right]^2 - \left[\mathcal{R}_0(r)\right]^2, \tag{3.10}$$

where the raised dot denotes the usual scalar product.

It remains to appraise the matrix elements f_{jk} whenever a certain form of the potential function is prescribed. The series in (3.2) suggests evidently that $V(r, \eta)$ itself possesses also an expansion of the same form

$$V(r, \eta) = \sum_{i=0}^{\infty} \nu_i(r) T_i(\eta), \tag{3.11}$$

where the coefficients $\nu_i(r)$, given by

$$\nu_i(r) = \mathcal{N}_i^{-1} \int_{-1}^{1} V(r, \eta) T_i(\eta) \left(1 - \eta^2\right)^{-1/2} \mathrm{d}\eta, \tag{3.12}$$

may be referred to as the potential coefficients. We now encounter the evaluation of integrals of the type

$$f_{jk}(r) = \mathcal{N}_k^{-1} \sum_{i=0}^{\infty} \nu_i(r) \int_{-1}^{1} T_i(\eta) T_j(\eta) T_k(\eta) \left(1 - \eta^2\right)^{-1/2} \mathrm{d}\eta \tag{3.13}$$

upon substituting (3.11) into (3.3). Fortunately, the use of the truly nice identity for the Chebyshev polynomials [8]

$$2T_j(\eta) T_k(\eta) = T_{j+k}(\eta) + T_{j-k}(\eta), \quad k \leqslant j, \tag{3.14}$$

yields the possibility of expressing the matrix elements f_{jk} as simple combinations of the potential coefficients such that

$$f_{00}(r) = \nu_0(r), \qquad f_{j,0}(r) = \frac{1}{2}\nu_j(r), \qquad f_{jj}(r) = \nu_0(r) + \frac{1}{2}\nu_{2j}(r) \tag{3.15}$$

and that

$$f_{jk}(r) = \frac{1}{2}\big[\nu_{j+k}(r) + \nu_{j-k}(r)\big], \quad k = 1, 2, \ldots, j-1, \tag{3.16}$$

for $j = 1, 2, \ldots$. Then the elements of the matrix $[f_{jk}]$ above the diagonal are calculated by the relations in (3.4).

Note that this procedure is not dependent on $V(r, \eta)$ having an expansion of the specific form (3.11). As a matter of fact, all that is required is that the η-dependence of $V(r, \eta)$ should be such that the integrals in (3.3) are convergent. In particular, the potential function may consist of a finite number of terms in which r and η variations are separable, and η variation is expressible as a polynomial of a low degree. One such explicit example will be treated in the coming section.

4. A specimen application

The classical quartic anharmonic oscillator problem provides a convenient numerical testing ground for the present method. In two-dimensional Cartesian coordinates, the scaled quartic potential having the reflection and the interchange symmetries is given by

$$V(x, y) = v_2\big(x^2 + y^2\big) + v_4\big(x^4 + 2\alpha x^2 y^2 + y^4\big), \tag{4.1}$$

where $v_4 > 0$, v_2 and $\alpha \in [-1, 1]$ are the coupling constants [3]. This potential is written as

$$V(r, \theta) = v_2 r^2 + v_4 r^4\big[1 - 2(1-\alpha)\sin^2\theta\cos^2\theta\big] \tag{4.2}$$

in the cylindrical polar coordinates, which may be transformed into the form

$$V(r, \eta) = \nu_0(r) T_0(\eta) + \nu_4(r) T_4(\eta) \tag{4.3}$$

on using (2.4), where

$$\nu_0(r) = v_2 r^2 + v_4\left[1 - \frac{1}{4}(1-\alpha)\right] r^4, \qquad \nu_4(r) = \frac{1}{4}(1-\alpha) v_4 r^4. \tag{4.4}$$

It is clear that (4.3) containing only two terms is a special case of the series expansion of the potential function (3.11), in which the potential coefficients $\nu_i(r)$, except $\nu_0(r)$ and $\nu_4(r)$, all vanish. Notice also that, because of the symmetries of the potential, the matrix $\mathbf{f}(r)$ has only three non-zero diagonal entries $f_{jj}(r)$, $f_{j,j-4}(r)$ and $f_{j-4,j}(r)$, which are evaluated from (3.15), (3.16) and (3.4), respectively. Hence, the matrix differential operator $\mathbf{H}$ becomes

$$\mathbf{H} \triangleq [H_{jk}] = \begin{bmatrix} H_{00} & 0 & 0 & 0 & H_{04} & 0 & \dots & 0 & \dots \\ 0 & H_{11} & 0 & 0 & 0 & H_{15} & & \vdots & \\ 0 & 0 & H_{22} & 0 & 0 & 0 & \ddots & 0 & \\ 0 & 0 & 0 & H_{33} & 0 & 0 & & H_{j-4,j} & \\ H_{40} & 0 & 0 & 0 & H_{44} & 0 & & 0 & \ddots \\ 0 & H_{51} & 0 & 0 & 0 & H_{55} & & 0 & \\ \vdots & & \ddots & & & & \ddots & 0 & \\ 0 & \dots & 0 & H_{j,j-4} & 0 & 0 & 0 & H_{jj} & \\ \vdots & & & & \ddots & & & & \ddots \end{bmatrix}. \tag{4.5}$$

This structure of the specific problem being considered here implies the decomposition of the set of Chebyshev polynomials into four subsets

$$\{T_m(\eta)\} \triangleq \{\{T_{4m}(\eta)\}, \{T_{4m+1}(\eta)\}, \{T_{4m+2}(\eta)\}, \{T_{4m+3}(\eta)\}\}. \tag{4.6}$$

Thus, four independent expansions of the wavefunction into the subsets of Chebyshev polynomials such as

$$\Psi_i(r, \eta) = \sum_{m=0}^{\infty} \mathcal{R}_{4m+i}(r) T_{4m+i}(\eta), \quad i = 0, 1, 2, 3, \tag{4.7}$$

may be proposed, corresponding to energy levels with different parities. However, we deal only with the subset of the spectrum provided by the eigenfunctions of the form

$$\Psi_0(r, \eta) = \sum_{m=0}^{\infty} P_m(r) T_{4m}(\eta), \tag{4.8}$$

where

$$P_m(r) \triangleq \mathcal{R}_{4m}(r), \quad m = 0, 1, \dots, \tag{4.9}$$

without any loss of generality. Then the system of ODEs reduces to the tridiagonal form

$$\begin{bmatrix} \mathcal{G}_0 & g_{01} & 0 & \dots & 0 & \dots \\ g_{10} & \mathcal{G}_1 & g_{12} & \ddots & \vdots & \\ 0 & g_{21} & \mathcal{G}_2 & \ddots & 0 & \\ \vdots & \ddots & \ddots & \ddots & g_{m-1,m} & \\ 0 & \dots & 0 & g_{m,m-1} & \mathcal{G}_m & \ddots \\ \vdots & & & & \ddots & \ddots \end{bmatrix} \begin{bmatrix} P_0(r) \\ P_1(r) \\ P_2(r) \\ \vdots \\ P_m(r) \\ \vdots \end{bmatrix} = E \begin{bmatrix} P_0(r) \\ P_1(r) \\ P_2(r) \\ \vdots \\ P_m(r) \\ \vdots \end{bmatrix} \tag{4.10}$$

in which

$$\mathcal{G}_m = -\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \left(16m^2 - \frac{1}{4}\right)\frac{1}{r^2} + g_{mm}(r), \qquad g_{jk}(r) \triangleq f_{4j,4k}(r) \tag{4.11}$$

for all m, j and k.

To compute the eigenvalues of the quartic oscillator, a Rayleigh–Ritz type approach may be appropriate. If we consider the functions

$$\phi_n^{(s)}(r) = C_n^{(s)} r^{s+1/2} \mathrm{e}^{-r^2/2} L_n^{(s)}\big(r^2\big), \quad n = 0, 1, \ldots, \tag{4.12}$$

for some prescribed $s \in \mathbb{R}$, where the $L_n^{(s)}(x)$ and $C_n^{(s)}$,

$$C_n^{(s)} = \sqrt{\frac{2n!}{\Gamma(s+n+1)}}, \tag{4.13}$$

are the associated Laguerre polynomials and a normalization factor, respectively, then the set

$$\big\{\phi_n^{(s)}(r)\big\} = \big\{\phi_0^{(s)}(r), \phi_1^{(s)}(r), \ldots, \phi_n^{(s)}(r), \ldots\big\} \tag{4.14}$$

comprises an orthonormal basis over $r \in [0, \infty)$. The basis functions so defined satisfy the classical harmonic oscillator Hamiltonian

$$\left[-\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \left(s^2 - \frac{1}{4}\right)\frac{1}{r^2} + r^2\right]\phi_n^{(s)}(r) = 2(2n+s+1)\phi_n^{(s)}(r) \tag{4.15}$$

on the semi-infinite line.

The asymptotic forms of the $P_m(r)$ displayed in propositions 2 and 3 are reflected by such a Laguerre basis when $s = 4m$, which justifies *a priori* the truncated approximate solution for each m

$$P_m(r) \simeq \sum_{n=0}^{N-1} p_n^{(m)} \phi_n^{(4m)}(r), \quad m = 0, 1, \ldots, M-1, \tag{4.16}$$

to be proposed at the numerical side of this work. It should be noted that the infinite system of ODEs in (4.10) is also truncated to M equations while N stands for the number of basis elements considered in the expansion of $P_m(r)$. Now the application of standart techniques reduces the system of ODEs to a matrix eigenvalue problem to determine the coefficients $p_n^{(m)}$ in (4.16), which may be regarded as N-vectors of the form

$$\mathbf{p}_m \triangleq \big[p_n^{(m)}\big] \triangleq \big[p_0^{(m)}, p_1^{(m)}, \ldots, p_{N-1}^{(m)}\big]^{\mathrm{T}} \tag{4.17}$$

for each $m = 0, 1, \ldots, M-1$. More specifically, the MN (M times N) unknowns $p_n^{(m)}$ are related by MN Galerkin equations having the block tridiagonal structure

$$\begin{bmatrix} \mathbf{G}_0 & \mathbf{U}_1 & \mathbf{0} & \ldots & \mathbf{0} \\ \frac{1}{2}\mathbf{U}_1^{\mathrm{T}} & \mathbf{G}_1 & \mathbf{U}_2 & & \vdots \\ \mathbf{0} & \mathbf{U}_2^{\mathrm{T}} & \mathbf{G}_2 & \ddots & \mathbf{0} \\ \vdots & & \ddots & \ddots & \mathbf{U}_{M-1} \\ \mathbf{0} & \ldots & \mathbf{0} & \mathbf{U}_{M-1}^{\mathrm{T}} & \mathbf{G}_{M-1} \end{bmatrix} \begin{bmatrix} \mathbf{p}_0 \\ \mathbf{p}_1 \\ \mathbf{p}_2 \\ \vdots \\ \mathbf{p}_{M-2} \\ \mathbf{p}_{M-1} \end{bmatrix} = E \begin{bmatrix} \mathbf{p}_0 \\ \mathbf{p}_1 \\ \mathbf{p}_2 \\ \vdots \\ \mathbf{p}_{M-2} \\ \mathbf{p}_{M-1} \end{bmatrix}, \tag{4.18}$$

where the $N \times N$ symmetric matrices $\mathbf{G}_m$ on the diagonal and the matrices $\mathbf{U}_m$ on the subdiagonal are defined by

$$\mathbf{G}_m \triangleq \left[G_{ij}^{(m)}\right], \quad G_{ij}^{(m)} = 2(2i + 4m + 1)\delta_{ij} + (v_2 - 1)A_{ij}^{(m)} + \frac{1}{4}(3 + \alpha)v_4 B_{ij}^{(m)} \tag{4.19}$$

for $m = 0, 1, \ldots, M-1$, and

$$\mathbf{U}_m \triangleq \left[U_{ij}^{(m)}\right], \quad U_{ij}^{(m)} = \frac{1}{8}(1 + \delta_{m,1})(1 - \alpha)v_4 \sum_{k=0}^{\min\{j,4\}} (-1)^k \binom{4}{k} \frac{C_j^{(4m-4)}}{C_{j-k}^{(4m)}} \delta_{i,j-k} \tag{4.20}$$

for $m = 1, \ldots, M-1$, respectively. Notice that the matrix elements are formulated in a concise manner by making use of the basic relationships satisfied by the associated Laguerre polynomials [10]. Moreover, the terms $A_{ij}^{(m)}$ and $B_{ij}^{(m)}$ in (4.19) stand for the integrals

$$A_{ij}^{(m)} = \int_0^\infty r^2 \phi_i^{(4m)}(r)\phi_j^{(4m)}(r)\,\mathrm{d}r \tag{4.21}$$

and

$$B_{ij}^{(m)} = \int_0^\infty r^4 \phi_i^{(4m)}(r)\phi_j^{(4m)}(r)\,\mathrm{d}r, \tag{4.22}$$

respectively, which can be evaluated analytically as well. As is shown immediately, the coefficient matrix in (4.18) has a non-symmetric structure even though the matrices $\mathbf{G}_m$ on the main diagonal are all symmetric.

5. Numerical results and discussion

The computational problem established in section 4 presents a two-dimensional array of approximations, say $[M, N]$. On the one hand, the size of the system (4.10) of ODEs, denoted by the number of equations M, can be extended to more precisely characterize the wavefunction $\Psi_0(r, \eta)$. On the other hand, the truncation order N is another adjustable parameter to represent each Fourier coefficient $P_m(r)$ to a desired accuracy. Therefore, computer experiments over the approximations $[M, N]$ are performed systematically to realize the numerical features of the algorithm. From a scientific com-

Table 1
The convergence rates of the first two eigenvalues in the near harmonic regime, where $v_2 = 1$, $v_4 = 10^{-3}$, as a function of α.

α	$[M, N]$	E_{00}	E_{01}
-1	[1, 4]	2.000 998 877	6.006 983 950
	[1, 5]	2.000 998 877	6.006 983 950
	[2, 7]	2.000 998 505 470	6.006 970 242 192
	[2, 8]	2.000 998 505 470	6.006 970 242 192
	[3, 7]	2.000 998 505 469 810	6.006 970 242 132 821
	[3, 8]	2.000 998 505 469 810	6.006 970 242 132 821
	[4, 8]	2.000 998 505 469 810	6.006 970 242 132 821
0	[1, 4]	2.001 497 478	6.010 463 971
	[1, 5]	2.001 497 478	6.010 463 971
	[2, 6]	2.001 497 385 346 390	6.010 460 565 464
	[2, 7]	2.001 497 385 346 389	6.010 460 565 464
	[3, 7]	2.001 497 385 346 371	6.010 460 565 461 293
	[3, 8]	2.001 497 385 346 371	6.010 460 565 461 293
	[4, 8]	2.001 497 385 346 371	6.010 460 565 461 293
1	[1, 6]	2.001 995 522 094 708	6.013 936 098 189 659
	[1, 7]	2.001 995 522 094 708	6.013 936 098 189 653
	[2, 7]	2.001 995 522 094 708	6.013 936 098 189 653
	[3, 7]	2.001 995 522 094 708	6.013 936 098 189 653

putational viewpoint, to determine the eigenvalues of a system of ODEs like (4.10) to a high accuracy is not immaterial. It is also noteworthy that a very similar system is encountered in the study of the few-body Schrödinger equation wherein the so-called coupling potential matrix is replaced by our **f** matrix [11].

We treat the cases specified by the set of constants

$$\{v_2, \alpha, v_4\} = \left\{\{1\}, \{-1, 0, 1\}, \left\{10^{-3}, 1, \infty\right\}\right\} \tag{5.1}$$

in the model potential (4.1). More clearly, the harmonic constant v_2 is set to unity without any loss of generality, since a linear scaling transformation maps any case to $v_2 = 1$. We choose the values of 0 and 1 of the parameter α, showing the interaction between x and y, or r and θ, coordinates, in order to examine two degenerate cases of considering, respectively, two independent quartic oscillators and a central potential. In fact, such degenerate potentials can be characterized by one-dimensional problems, which are useful for a numerical comparison with the other methods. The three values of the anharmonicity constant v_4 correspond to three distinct regimes of the eigenvalues; namely, the near harmonic, the boundary layer and the pure anharmonic levels.

The numerical results shown in tables 1–3 demonstrate the calculation of the first two energy levels as the limit of converging sequences. The finally reported eigenvalues accurate to 16 significant figures are in excellent agreement with the previously published data [12].

Table 2
The convergence rates of the first two eigenvalues in the boundary layer regime, where $v_2 = v_4 = 1$, as a function of α.

α	$[M, N]$	E_{00}	E_{01}
-1	[2, 14]	2.563	8.52
	[5, 17]	2.561 626 664	8.436 034
	[8, 20]	2.561 626 575 675	8.435 987 355
	[10, 28]	2.561 626 575 640 188	8.435 987 322 637
	[12, 34]	2.561 626 575 640 033	8.435 987 322 352
	[15, 38]	2.561 626 575 640 032	8.435 987 322 348 472
	[16, 40]	2.561 626 575 640 032	8.435 987 322 348 468
	[16, 42]	2.561 626 575 640 032	8.435 987 322 348 468
	[17, 42]	2.561 626 575 640 032	8.435 987 322 348 467
0	[2, 15]	2.784 715	10.048
	[4, 20]	2.784 703 283 185	10.047 401 623
	[6, 32]	2.784 703 283 060 586	10.047 401 599 289 96
	[7, 35]	2.784 703 283 060 584	10.047 401 599 289 61
	[7, 36]	2.784 703 283 060 584	10.047 401 599 289 61
	[8, 38]	2.784 703 283 060 584	10.047 401 599 289 60
1	[2, 20]	2.952 050 092 126	10.882 435 590
	[4, 30]	2.952 050 091 962 893	10.882 435 576 829
	[6, 36]	2.952 050 091 962 874	10.882 435 576 819 84
	[6, 38]	2.952 050 091 962 874	10.882 435 576 819 82
	[7, 40]	2.952 050 091 962 874	10.882 435 576 819 81

Note that $v_4 \to \infty$ limit in table 3 represents the pure quartic oscillator problem, the treatment of which can be accomplished if $V(r, \eta)$ and E in (3.1) are replaced by

$$V(r, \eta) = \left\{1 + \frac{1}{4}(1 - \alpha)\big[T_4(\eta) - 1\big]\right\} r^4 \tag{5.2}$$

and $\mathcal{E}$, respectively, where $E = \mathcal{E} v_4^{1/3}$. In other words, the total energy E grows like $\mathcal{E} v_4^{1/3}$ as $v_4 \to \infty$, and table 3 lists the coefficient $\mathcal{E}$ in this asymptotic relation.

Owing to the harmonic nature of the basis functions (4.12), however, it is not difficult to anticipate the convergence slowdown in the pure anharmonic and, partially, in the boundary layer regimes. Evidently, the prescribed accuracy can be attained at the cost of employing higher approximation orders such as $[M, N] = [30, 60]$. To accelerate the convergence in the anharmonic regimes, a superfluous parameter might have been inserted into the algorithm, and we had tried for its optimum values. But the use of such numerical tricks is outside the scope of this article. Nevertheless, the present method is superior to classical variational schemes wherein the diagonalization of $N^2 \times N^2$ matrices necessitate inevitably. It is observed from the recorded material that the approximations $[M, N]$ stabilize when $M < N$ leading to matrices of sizes $MN \times MN$ less than $N^2 \times N^2$. That is, the achievement of accuracy and of stability does not require necessarily the inspection of approximations $[N, N]$ along the diagonal sequence. In fact,

Table 3
The convergence rates of the first two eigenvalues in the pure anharmonic regime, where $v_2 = 1$, $v_4 \to \infty$, as a function of α.

α	$[M, N]$	$v_4^{-1/3} E_{00}$	$v_4^{-1/3} E_{01}$
-1	[2, 15]	1.768	6.2
	[5, 15]	1.759 213	5.592
	[10, 25]	1.759 194 609 370	5.579 649
	[15, 40]	1.759 194 606 177	5.579 633 841
	[18, 45]	1.759 194 606 175 558	5.579 633 812 907
	[20, 50]	1.759 194 606 175 533	5.579 633 812 131
	[25, 55]	1.759 194 606 175 533	5.579 633 812 124 029
	[28, 60]	1.759 194 606 175 533	5.579 633 812 123 763
	[30, 60]	1.759 194 606 175 533	5.579 633 812 123 753
0	[2, 10]	2.120 764	8.517
	[4, 18]	2.120 724 182	8.516 060 140
	[6, 25]	2.120 724 180 969	8.516 060 028 567
	[7, 32]	2.120 724 180 968 367	8.516 060 028 471
	[8, 35]	2.120 724 180 968 366	8.516 060 028 470 937
	[8, 37]	2.120 724 180 968 366	8.516 060 028 470 922
	[9, 38]	2.120 724 180 968 366	8.516 060 028 470 921
1	[1, 18]	2.344 829 075	9.529 781 482
	[2, 22]	2.344 829 072 850	9.529 781 395
	[3, 26]	2.344 829 072 744 847	9.529 781 384 227
	[4, 34]	2.344 829 072 744 276	9.529 781 384 015 208
	[5, 40]	2.344 829 072 744 275	9.529 781 384 014 809
	[5, 42]	2.344 829 072 744 275	9.529 781 384 014 809
	[6, 44]	2.344 829 072 744 275	9.529 781 384 014 808

the sequence of approximations $[M, N]$ pertaining to the Mth row may successfully converge to the desired eigenvalue.

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