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Research Article

The Laguerre pseudospectral method for the two-dimensional Schrödinger equation with symmetric nonseparable potentials

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Abstract

The Hermite pseudospectral method is one of the natural techniques for the numerical treatment of the problems defined over unbounded domains such as two-dimensional time-independent Schrödinger equation on the whole real plane. However, it is shown here that for the symmetric potentials, transformation of the problem over the first quadrant and the application of the Laguerre pseudospectral method reduce the cost by a factor of four when compared to the Hermite pseudospectral method.

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1. Introduction

In [1], the eigenvalues and wavefunctions of the two-dimensional time-independent Schrödinger equation

$$\left[-\frac{\partial^2}{\partial x^2}-\frac{\partial^2}{\partial y^2}+V(x,y)\right]\Psi(x,y)=E\Psi(x,y),\quad (x,y)\in\mathbb{R}^2 \tag{1.1}$$

with the boundary conditions

$$\begin{aligned}\Psi(x,\pm\infty)&=0,\quad -\infty<x<\infty\\ \Psi(\pm\infty,y)&=0,\quad -\infty<y<\infty\end{aligned} \tag{1.2}$$

are approximated by means of the Hermite pseudospectral method (HPM) for several nonseparable quantum mechanical potentials $V(x,y)$. In this article, we consider the reflection symmetric potentials

$$V(x,y)=V(-x,y)=V(x,-y)=V(-x,-y) \tag{1.3}$$

for which the spectrum of the system (1.1)-(1.2) can be decomposed into four subsets containing the states $E_{2n,2m}$, $E_{2n,2m+1}$, $E_{2n+1,2m}$ and $E_{2n+1,2m+1}$. Although the Hermite pseudospectral method can still be used with further modifications in the Lagrange interpolant so that each eigenvalue subset can be treated by a separate basis set, it does not seem practical. Therefore, the main aim of this paper is to find more natural basis sets which can treat the states $E_{2n,2m}$, $E_{2n,2m+1}$, $E_{2n+1,2m}$ and $E_{2n+1,2m+1}$ separately. In this

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case, one deals with four matrices of size $N^2 \times N^2$ instead of a matrix of size $(2N)^2 \times (2N)^2$ reducing the cost by a factor of two in each direction which is a considerable amount in two dimensions.

First of all the reflection symmetric character of the potential suggests the use of transformations

$$\xi = (\alpha x)^2, \quad \eta = (\alpha y)^2, \quad \alpha > 0 \tag{1.4}$$

where the parameter α may be regarded as an optimization parameter and introduced for numerical purposes. With (1.4), the Schrödinger equation takes the form

$$\left[\xi \frac{\partial^2}{\partial \xi^2} + \eta \frac{\partial^2}{\partial \eta^2} + \frac{1}{2}\frac{\partial}{\partial \xi} + \frac{1}{2}\frac{\partial}{\partial \eta} - \frac{1}{4\alpha^2} V\left(\sqrt{\xi}/\alpha, \sqrt{\eta}/\alpha\right)\right] \Psi = -\frac{E}{4\alpha^2}\Psi \tag{1.5}$$

where $(\xi, \eta) \in (0, \infty) \times (0, \infty)$. Accordingly the boundary conditions in (1.2) read as

$$\begin{aligned} &\Psi(\xi, \infty) = 0, \quad 0 < \xi < \infty \\ &\Psi(\infty, \eta) = 0, \quad 0 < \eta < \infty. \end{aligned} \tag{1.6}$$

Now, introducing the transformation

$$\Psi(\xi, \eta) = \xi^{s_1} \eta^{s_2} e^{-\frac{1}{2}(\xi+\eta)} \Phi(\xi, \eta), \quad s_1,\, s_2 \geq 0 \tag{1.7}$$

satisfying the boundary conditions in (6) where the polynomial terms are introduced to cope with the artificial singularity at $\xi = 0$ and $\eta = 0$, we rewrite the last equation as

$$\left[\xi \frac{\partial^2}{\partial \xi^2} + \eta \frac{\partial^2}{\partial \eta^2} + \left(2s_1 + \tfrac{1}{2} - \xi\right)\frac{\partial}{\partial \xi} + \left(2s_2 + \tfrac{1}{2} - \eta\right)\frac{\partial}{\partial \eta} + Q\right] \Phi = \mathcal{E}\Phi \tag{1.8}$$

where

$$Q = \frac{s_1(s_1 - 1/2)}{\xi} + \frac{s_2(s_2 - 1/2)}{\eta} + \frac{\xi + \eta}{4} - \frac{1}{4\alpha^2} V\left(\sqrt{\xi}/\alpha, \sqrt{\eta}/\alpha\right) \tag{1.9}$$

stands for the modified potential and

$$\mathcal{E} = \mathcal{E}(s_1, s_2, \alpha) = s_1 + s_2 + \frac{1}{2} - \frac{E}{4\alpha^2} \tag{1.10}$$

the shifted eigenvalues. Notice from (1.7) that the new dependent variable Φ does not have to satisfy any boundary condition as long as it is a bounded function of ξ and η.

Then, to get rid of the unwelcome terms that are proportional to ξ^{-1} and η^{-1} appearing in the modified potential, we are free to choose any one of the elements from the set $\left\{(0,0), (0, \frac{1}{2}), (\frac{1}{2}, 0), (\frac{1}{2}, \frac{1}{2})\right\}$ for (s_1, s_2). Moreover, setting

$$2s_i + \frac{1}{2} = \gamma_i + 1, \quad i = 1, 2 \tag{1.11}$$

the last equation reads as

$$\left[\xi \frac{\partial^2}{\partial \xi^2} + \eta \frac{\partial^2}{\partial \eta^2} + (\gamma_1 + 1 - \xi)\frac{\partial}{\partial \xi} + (\gamma_2 + 1 - \eta)\frac{\partial}{\partial \eta} + Q\right] \Phi = \mathcal{E}\Phi \tag{1.12}$$

where the modified potential

$$Q = Q(\xi, \eta; \alpha) = \frac{1}{4}\left[\xi + \eta - \frac{1}{\alpha^2} V\left(\sqrt{\xi}/\alpha, \sqrt{\eta}/\alpha\right)\right] \tag{1.13}$$

is now free of the parameters γ_i, and hence s_i, for $i = 1, 2$. Meanwhile, the shifted eigenvalues becomes

$$\mathcal{E} = \mathcal{E}(\gamma_1, \gamma_2, \alpha) = \frac{1}{2}(\gamma_1 + \gamma_2) + 1 - \frac{E}{4\alpha^2}. \tag{1.14}$$

Notice from (1.7) that the $(\gamma_1, \gamma_2) \in \left\{(-\frac{1}{2}, -\frac{1}{2}), (-\frac{1}{2}, \frac{1}{2}), (\frac{1}{2}, -\frac{1}{2}), (\frac{1}{2}, \frac{1}{2})\right\}$ values obtained from (1.11) lead to the states $E_{2m,2n}$, $E_{2m,2n+1}$, $E_{2m+1,2n}$ and $E_{2m+1,2n+1}$ respectively. This can be seen on returning back to the original variables (x, y) via (1.4).

Note that the Schrödinger equation in (1.1) is defined over the whole real plane whereas the transformed equation (1.12) of a reflection symmetric system is defined over the first quadrant. Thus, the direct application of the HPM used in [1] is not possible anymore. Instead, Laguerre pseudospectral method (LPM) seems more feasible since the Laguerre polynomials constitute a complete orthogonal set on the half line $(0, \infty)$.

Therefore, in section 2 we construct the pseudospectral formulation of the transformed equation in (1.12) based on the Laguerre polynomials. Section 3 includes numerical examples and some implementation notes. The last section concludes the paper with some remarks.

2. Pseudospectral formulation of the problem

Since a pseudospectral method is based on a polynomial interpolation in the Lagrange form, we propose an approximate solution of the form

$$\Phi(\xi,\eta) = \sum_{n=0}^{N}\sum_{j=0}^{N} \ell_n(\xi)\ell_j(\eta)\Phi_{nj} \tag{2.1}$$

where

$$\ell_k(\xi) = \frac{\phi_{N+1}(\xi)}{(\xi-\xi_k)\phi'_{N+1}(\xi_k)}, \quad k = 0, 1, \ldots, N \tag{2.2}$$

are the set of N-th degree Lagrange interpolating polynomials in which

$$\phi_{N+1}(\xi) = k_{N+1}\prod_{i=0}^{N}(\xi-\xi_i), \quad k_{N+1} \in \mathbb{R} \tag{2.3}$$

is the $(N+1)$-st degree polynomial having real and distinct zeros. Here, $\Phi_{nj} = \Phi(\xi_n, \eta_j)$ are the exact values of $\Phi(\xi,\eta)$ at the specified grid points (ξ_n, η_j) for $n, j = 0, 1, \ldots, N$. Now to approximate the eigenvalues of the Schrödinger equation with symmetric potentials we set

$$\phi^{\gamma}_{N+1}(t) = \frac{L^{\gamma}_{N+1}(t)}{h_{N+1}}, \quad h^2_k = \frac{\Gamma(k+\gamma+1)}{k!}, \quad t \in (0,\infty) \tag{2.4}$$

in which $L^{\gamma}_{N+1}(t)$ is the Laguerre polynomial of degree $N+1$ and order $\gamma = \pm\frac{1}{2}$. Approximating the solutions of differential equations by Laguerre polynomials are usually not stable for large N due to their wild behaviors at infinity, and hence, one usually works with the Laguerre functions $\hat{L}^{\gamma}_N(t) = e^{-t/2}L^{\gamma}_N(t)$ instead. This situation is theoretically investigated, for example in [5, 7–9], and it is shown that the Laguerre functions have better stability properties than Laguerre polynomials. In this study, we search for the square integrable solutions of (1.1) which vanish exponentially at infinity. Therefore, the Laguerre functions are suitable for the numerical treatment of (1.1). But, since we factor off the term $e^{-(\xi+\eta)/2}$ from the solution by means of the transformation in (1.7), the use of Laguerre polynomials for equation (1.12) is equivalent to the use of Laguerre functions for the original problem in (1.1). Thus, we continue with the normalized Laguerre polynomials in (2.4) to approximate the eigenvalues of (1.12) and hence, those of the original equation in (1.1).

By (2.4) the grid points (ξ_n, η_j) are set to be the cartesian product of the zeros ξ_n and η_j of the Laguerre polynomials $L^{\gamma_1}_{N+1}(\xi)$ and $L^{\gamma_2}_{N+1}(\eta)$, respectively. That is, we have four set of grid points according to the choice of the parameters

$$(\gamma_1,\gamma_2) \in \left\{(-\frac{1}{2},-\frac{1}{2}),(-\frac{1}{2},\frac{1}{2}),(\frac{1}{2},-\frac{1}{2}),(\frac{1}{2},\frac{1}{2})\right\}$$

which will be used to approximate the states $E_{2m,2n}$, $E_{2m,2n+1}$, $E_{2m+1,2n}$ and $E_{2m+1,2n+1}$ respectively.

On the other hand, zeros of the normalized Laguerre polynomials may be determined to a desired accuracy as the eigenvalues of the tridiagonal matrix

$$\mathbf{R} = \begin{bmatrix} B_0 & A_1 & & & 0 \\ A_1 & B_1 & A_2 & & \\ & A_2 & B_2 & \ddots & \\ & & \ddots & \ddots & A_N \\ 0 & & & A_N & B_N \end{bmatrix} \tag{2.5}$$

where the $A_n = -\sqrt{n(n+\gamma)}$ and $B_n = 2n+\gamma+1$ are the coefficients in the three term recursion

$$A_{n+1}\phi^{\gamma}_{n+1}(\xi) + (B_n - \xi)\phi^{\gamma}_n(\xi) + A_n\phi^{\gamma}_{n-1}(\xi) = 0, \quad n = 0, 1, \dots \tag{2.6}$$

of the normalized Laguerre polynomials [2, 12]. Actually, the matrix $\mathbf{R}$ is obtained by running the recursion from $n = 0$ to $n = N$ and setting $\phi_{N+1}(\xi)$ to zero. Thus, the mth computed eigenvector $\mathbf{r}_m = [r_{0,m}\ r_{1,m}\ \dots\ r_{N-1,m}\ r_{N,m}]^T$ of $\mathbf{R}$ corresponding to the $m-$th eigenvalue (or root) ξ_m is a constant multiple of the vector of orthonormal polynomial values $\phi^{\gamma\ m} = [\phi^{\gamma}_0(\xi_m)\ \phi^{\gamma}_1(\xi_m)\ \dots\ \phi^{\gamma}_{N-1}(\xi_m)\ \phi^{\gamma}_N(\xi_m)]^T$ at the point ξ_m. That is, $\mathbf{r}_m = a\phi^m$. This constant may be determined by comparing the first elements $r_{0,m}$ and $\phi^{\gamma}_0(\xi_m)$ of these two vectors since $\phi^{\gamma}_0(\xi_m) = 1/h_0 = 1/\sqrt{\Gamma(\gamma+1)}$ is a constant. Therefore, for $n = 0, 1, \dots, N$, the values $\phi^{\gamma}_n(\xi_m)$ of the normalized classical orthogonal polynomials at the zeros of $\phi^{\gamma}_{N+1}(\xi)$ may be computed as

$$[\phi^{\gamma}_0(\xi_m)\ \phi^{\gamma}_1(\xi_m)\ \dots\ \phi^{\gamma}_{N-1}(\xi_m)\ \phi^{\gamma}_N(\xi_m)]^T = \frac{1}{\sqrt{\Gamma(\gamma+1)}r_{0,m}}[r_{0,m}\ r_{1,m}\ \dots\ r_{N-1,m}\ r_{N,m}]^T \tag{2.7}$$

in terms of the computed eigenvector $\mathbf{r}_m$ of tridiagonal symmetric matrix $\mathbf{R}$ of size $N+1$.

It is known as the Golub-Welsch algorithm whose details may be found, for example, in [2,4]. This procedure, unfortunately, suffers from computing the full set of eigenvalues with a uniform accuracy especially for large values of N. Therefore, in this case, alternative root finding algorithms, for example, Newton method may be used to compute the roots. Nevertheless, for moderate N values the Golub-Welsch algorithm can be used without any hesitation.

After determining the mesh points (ξ_n, η_j), we insert the approximate solution in (2.1) into the equation (1.12) and require its satisfaction at the grid points (ξ_m, η_i) to obtain the set of $(N+1)^2$ equations

$$\sum_{n=0}^{N}\sum_{j=0}^{N}[\widehat{L}_n(\xi_m)\ell_j(\eta_i) + \widehat{L}_j(\eta_i)\ell_n(\xi_m) + Q(\xi_m,\eta_i;\alpha)\ell_n(\xi_m)\ell_j(\eta_i)]\Phi_{nj} = \mathcal{E}(\gamma_1,\gamma_2,\alpha)\sum_{n=0}^{N}\sum_{j=0}^{N}\ell_n(\xi_m)\ell_j(\eta_i)\Phi_{nj} \tag{2.8}$$

for $m, i = 0, 1, \dots, N$ where

$$\widehat{L}_r(\zeta_p) := \widehat{L}^{\gamma}_{pr} = \zeta_p\ell''_r(\zeta_p) + (\gamma+1-\zeta_p)\ell'_r(\zeta_p). \tag{2.9}$$

Here, notice the dependence of the roots to the order γ of the Laguerre polynomials. That is, the points $\zeta_p := \zeta^{\gamma}_p$ are the roots of the $(N+1)$st degree Laguerre polynomials of order γ.

Therefore, by using (2.9) and the well-known property $\ell_r(\zeta_p) = \delta_{pr}$ of the Lagrange polynomials, the algebraic equations in (2.8) reads as

$$\sum_{n=0}^{N}\sum_{j=0}^{N}\left(\widehat{L}_{mn}^{\gamma_1}\delta_{ij} + \widehat{L}_{ij}^{\gamma_2}\delta_{mn} + Q_{mi}\delta_{mn}\delta_{ij}\right)\Phi_{nj} = \mathcal{E}(\gamma_1,\gamma_2,\alpha)\sum_{n=0}^{N}\sum_{j=0}^{N}\delta_{mn}\delta_{ij}\Phi_{nj} \quad (2.10)$$

where the $Q_{mi} = Q(\xi_m, \eta_i; \alpha)$ are the known values of the modified potential in (1.13) at the mesh points. The last equation may be written in the matrix-vector form

$$\widehat{\mathbf{B}}\mathbf{\Phi} = \mathcal{E}(\gamma_1,\gamma_2,\alpha)\mathbf{\Phi} \quad (2.11)$$

where

$$\widehat{\mathbf{B}}(\gamma_1,\gamma_2) := \widehat{\mathbf{B}} = \widehat{\mathbf{L}}^{\gamma_1}\otimes\mathbf{I} + \mathbf{I}\otimes\widehat{\mathbf{L}}^{\gamma_2} + \mathbf{Q_1} \quad (2.12)$$

is a matrix of dimension $(N+1)^2\times(N+1)^2$. Here $\mathbf{\Phi}$ is an $(N+1)^2\times 1$ vector containing the vectorized unknown wavefunction values at the grid points in the order

$$\mathbf{\Phi} = \left[\Phi_{00}\ \ldots\ \Phi_{0N}\ \Phi_{10}\ \ldots\ \Phi_{1N}\ \ldots\ \ldots\ \Phi_{N0}\ \ldots\ \Phi_{NN}\right]^T \quad (2.13)$$

where Φ_{ij} stand for the values $\Phi(\xi_i,\eta_j)$ of the wavefunction at the nodal points (ξ_i,η_j). Moreover, $\widehat{\mathbf{L}}^{\gamma_i}$ for $i=1,2$ stands for the kinetic energy matrix with entries (2.9), $\mathbf{I}$ the $(N+1)\times(N+1)$ identity matrix, $\mathbf{Q}$ the diagonal potential matrix whose diagonal entries contain the values $Q(\xi_m,\eta_i;\alpha)$ in the order specified in (2.13) and $\mathbf{M}_1\otimes\mathbf{M}_2$ the Kronecker product of the matrices $\mathbf{M_1}$ and $\mathbf{M}_2$.

The explicit entries [12]

$$\widehat{L}_{pr}^{\gamma} = -\frac{1}{6}\begin{cases}\dfrac{12\zeta_p}{(\zeta_p-\zeta_r)^2}\dfrac{\phi_{N+1}^{\gamma\,\prime}(\zeta_p)}{\phi_{N+1}^{\gamma\,\prime}(\zeta_r)} & \text{if } p\neq r\\[2ex] 2N+\dfrac{1}{\zeta_r}\left[(\gamma-\zeta_r)^2-1\right] & \text{if } p=r\end{cases} \quad (2.14)$$

of the matrix $\widehat{\mathbf{L}}^{\gamma}$ in (2.9) reveal that it is, and hence $\widehat{\mathbf{B}}$, is not symmetric. However, fortunately, the similarity transformation

$$\mathbf{L}^{\gamma} = (\mathbf{S}^{\gamma})^{-\mathbf{1}}\widehat{\mathbf{L}}^{\gamma}\mathbf{S}^{\gamma} \quad (2.15)$$

in which

$$\mathbf{S}^{\gamma} = s_p\delta_{pr} = \sqrt{\zeta_p}\phi_{N+1}^{\gamma\,\prime}(\zeta_p)\delta_{pr} \quad (2.16)$$

is a diagonal matrix symmetrizes the matrix $\widehat{\mathbf{L}}^{\gamma}$. In this case, the entries of the symmetric matrix $\mathbf{L}^{\gamma}$ reads as

$$L_{pr}^{\gamma} = -\frac{1}{6}\begin{cases}\dfrac{12\sqrt{\zeta_p\zeta_r}}{(\zeta_p-\zeta_r)^2} & \text{if } p\neq r\\[2ex] 2N+\dfrac{1}{\zeta_r}\left[(\gamma-\zeta_r)^2-1\right] & \text{if } p=r\end{cases} \quad (2.17)$$

with $K_{pr}^{\gamma} = K_{rp}^{\gamma}$. Therefore, we may state the following proposition.

Proposition 2.1. *The matrix*

$$\mathbf{T} = \mathbf{S}^{\gamma_1}\otimes\mathbf{S}^{\gamma_2} \quad (2.18)$$

in which $\mathbf{S}^{\gamma}$ *is given by (2.16), symmetrizes the matrix* $\widehat{\mathbf{B}}$ *in (2.12).*

Proof. By using the basic linear algebra tools

$$(\mathbf{A}\otimes\mathbf{B})^{-1}=\mathbf{A}^{-1}\otimes\mathbf{B}^{-1}\quad\text{and}\quad(\mathbf{A}\otimes\mathbf{B})(\mathbf{C}\otimes\mathbf{D})=\mathbf{AC}\otimes\mathbf{BD}\tag{2.19}$$

and after a little algebra we end up with

$$\begin{aligned}\mathbf{B}=\mathbf{T}^{-1}\widehat{\mathbf{B}}\mathbf{T}&=(\mathbf{S}^{\gamma_1}\otimes\mathbf{S}^{\gamma_2})^{-1}\left(\widehat{\mathbf{L}}^{\boldsymbol{\gamma_1}}\otimes\mathbf{I}+\mathbf{I}\otimes\widehat{\mathbf{L}}^{\boldsymbol{\gamma_2}}+\mathbf{Q}\right)(\mathbf{S}^{\gamma_1}\otimes\mathbf{S}^{\gamma_2})\\&=(\mathbf{S}^{\gamma_1})^{-1}\widehat{\mathbf{L}}^{\boldsymbol{\gamma_1}}\mathbf{S}^{\gamma_1}\otimes\mathbf{I}+\mathbf{I}\otimes(\mathbf{S}^{\gamma_2})^{-1}\widehat{\mathbf{L}}^{\boldsymbol{\gamma_2}}\mathbf{S}^{\gamma_2}\\&\quad+(\mathbf{S}^{\boldsymbol{\gamma_1}}\otimes\mathbf{S}^{\boldsymbol{\gamma_2}})^{-\mathbf{1}}\,\mathbf{Q}\,(\mathbf{S}^{\boldsymbol{\gamma_1}}\otimes\mathbf{S}^{\boldsymbol{\gamma_2}}).\end{aligned}$$

Now using (2.15) for the first two term and keeping in mind that $\mathbf{T}=\mathbf{S}^{\boldsymbol{\gamma_1}}\otimes\mathbf{S}^{\boldsymbol{\gamma_2}}$ and $\mathbf{Q}$ are diagonal matrices the last equation reads as

$$\mathbf{B}=\mathbf{L}^{\boldsymbol{\gamma_1}}\otimes\mathbf{I}+\mathbf{I}\otimes\mathbf{L}^{\boldsymbol{\gamma_2}}+\mathbf{Q}.\tag{2.20}$$

Hence, being the addition of symmetric matrices, $\mathbf{B}$ is symmetric. □

Thus we may replace the unsymmetrical system in (2.11) with the simple symmetric one

$$\mathbf{Bu}=\mathcal{E}\mathbf{u}\tag{2.21}$$

since the similar matrices participate of the same eigenvalue set. It is simple in the sense that the unpleasant term $\phi'_{N+1}(\zeta_p)/\phi'_{N+1}(\zeta_r)$ in (2.14) is removed by the similarity transformation in (2.18). Notice that the eigenvectors of the unsymmetrical and symmetric systems are linked as

$$\mathbf{\Phi}=\mathbf{Tu}\tag{2.22}$$

since $\mathbf{Bu}=\mathbf{T}^{-1}\widehat{\mathbf{B}}\mathbf{Tu}=\mathcal{E}\mathbf{u}$ implies $\widehat{\mathbf{B}}[\mathbf{Tu}]=\mathcal{E}[\mathbf{Tu}]$. The last equation may be written in nodal form as

$$\Phi(\xi_m,\eta_i)=\sqrt{\xi_m\eta_i}\phi_{N+1}^{\gamma_1\,\prime}(\xi_m)\phi_{N+1}^{\gamma_2\,\prime}(\eta_i)u_{mi}\tag{2.23}$$

with the help of (2.16) and (2.18). Then, (1.7) together with (1.11) and (2.23) leads to the values of the original wavefunction

$$\Psi(\xi_m,\eta_i)=\phi_{N+1}^{\gamma_1\,\prime}(\xi_m)\phi_{N+1}^{\gamma_2\,\prime}(\eta_i)\xi_m^{\frac{1}{2}(\gamma_1+\frac{3}{2})}\eta_i^{\frac{1}{2}(\gamma_2+\frac{3}{2})}e^{-\frac{1}{2}(\xi+\eta)}u_{mi}\tag{2.24}$$

at the mesh point (ξ_m,η_i) in terms of an eigenvector $\mathbf{u}$ of (2.21). On the other hand, setting $n=N+1$ and $x=\xi_m,\eta_i$ in the differential difference relation

$$x\phi_n^{\gamma\,\prime}(x)=n\phi_n^{\gamma\,\prime}(x)-\sqrt{n(n+\gamma)}\phi_{n-1}^{\gamma\,\prime}(x)\tag{2.25}$$

of the normalized Laguerre polynomials we obtain

$$\begin{aligned}\xi_m\phi_{N+1}^{\gamma_1\,\prime}(\xi_m)&=-\sqrt{(N+1)(N+\gamma_1+1)}\phi_N^{\gamma_1}(\xi_m)\\\eta_i\phi_{N+1}^{\gamma_2\,\prime}(\eta_i)&=-\sqrt{(N+1)(N+\gamma_2+1)}\phi_N^{\gamma_2}(\eta_i)\end{aligned}\tag{2.26}$$

since $\phi_{N+1}^{\gamma_1}(\xi_m)=\phi_{N+1}^{\gamma_2}(\eta_i)=0$. Now, using (2.7) and (2.26), equation (2.24) reads as

$$\Psi(\xi_m,\eta_i)=C(N,\gamma_1,\gamma_2)\frac{r_{N,m}}{r_{0,m}}\frac{r_{N,i}}{r_{0,i}}\xi_m^{\frac{1}{2}(\gamma_1-\frac{1}{2})}\eta_i^{\frac{1}{2}(\gamma_2-\frac{1}{2})}e^{-\frac{1}{2}(\xi_m+\eta_i)}u_{mi}\tag{2.27}$$

where

$$C(N,\gamma_1,\gamma_2)=(N+1)\sqrt{\frac{(N+\gamma_1+1)(N+\gamma_2+1)}{\Gamma(\gamma_1+1)\Gamma(\gamma_2+1)}}.\tag{2.28}$$

Now, we are in a position to state the following theorem:

Theorem 2.2. *The approximate eigenvalues E_k of the two-dimensional Schrödinger equation in (1.1) together with the boundary condition (1.2) are related with the eigenvalues $\mathcal{E}_k$ of the matrix $\mathbf{B}(\gamma_1,\gamma_2)$ in (2.21) by the formula*

$$E_k = 4\alpha^2\left[\frac{1}{2}(\gamma_1+\gamma_2)+1-\mathcal{E}_k(\gamma_1,\gamma_2,\alpha)\right], \qquad k=0,1,\ldots \tag{2.29}$$

and the values of the corresponding normalized eigenfunctions $\bar{\Psi}_k(x_n,y_j)$ (in L^2 sense) at the mesh points in the first quadrant $(x_n,y_j)=(\sqrt{\xi_n}/\alpha,\sqrt{\eta_j}/\alpha)$ are given by

$$\bar{\Psi}_k(x_m,y_i) = \alpha C(N,\gamma_1,\gamma_2)\frac{r_{N,m}}{r_{0,m}}\frac{r_{N,i}}{r_{0,i}}\xi_m^{\frac{1}{2}(\gamma_1-\frac{1}{2})}\eta_i^{\frac{1}{2}(\gamma_2-\frac{1}{2})}e^{-\frac{1}{2}(\xi_m+\eta_i)}u_{mi}^k \tag{2.30}$$

provided that $\boldsymbol{u}^k$ is the $k-th$ normalized (in Euclidean 2-norm) eigenvector of (2.21). Finally, the complete picture of the normalized eigenfunction $\bar{\Psi}_k(x,y)$ in the whole plane, at the original mesh points $(x_m,y_i)=(\pm\sqrt{\xi_n}/\alpha,\pm\sqrt{\eta_j}/\alpha)$ is obtained by appropriately (even and/or odd) extending the values in (2.30) *to the other quadrants.*

Proof. The first part easily follows from (1.10) and (1.11). For the second part, keeping in mind that for symmetric potentials the squares of the eigenfunctions are equal in all quadrants and then using the transformations in (1.4) and (1.7) we write

$$\begin{aligned}\left\|\bar{\Psi}_k\right\|_{L^2}^2 &= \int\int_{\mathbb{R}^2}\bar{\Psi}_k^2(x,y)\mathrm{d}x\mathrm{d}y = 4\int\int_{\mathbb{R}^{+^2}}\bar{\Psi}_k^2(x,y)\mathrm{d}x\mathrm{d}y\\ &= 4\alpha^2\int\int_{\mathbb{R}^{+^2}}\Psi_k^2(x,y)\mathrm{d}x\mathrm{d}y = 4\alpha^2\int\int_{\mathbb{R}^{+^2}}\Psi_k^2(\xi,\eta)\frac{1}{4\alpha^2\sqrt{\xi\eta}}\mathrm{d}\xi\mathrm{d}\eta\\ &= \int\int_{\mathbb{R}^{+^2}}\Phi_k^2(\xi,\eta)\xi^{\gamma_1}\eta^{\gamma_2}e^{-(\xi+\eta)}\mathrm{d}\xi\mathrm{d}\eta\end{aligned} \tag{2.31}$$

Now, applying the N+1 point Gauss-Laguerre quadrature to the last integral we have

$$\left\|\bar{\Psi}_k\right\|_{L^2}^2 = \lim_{N\to\infty}\sum_{m=0}^{N}\sum_{i=0}^{N}\Phi_k^2(\xi_m,\xi_i)\omega_m^{\gamma_1}\omega_i^{\gamma_2} \tag{2.32}$$

where

$$\begin{aligned}\omega_m^{\gamma_1} &= \frac{1}{(N+1)(N+\gamma_1+1)}\frac{\xi_m}{{\phi_N^{\gamma_1}}^2(\xi_m)}, \quad m=0,1,\ldots,N\\ \omega_i^{\gamma_2} &= \frac{1}{(N+1)(N+\gamma_2+1)}\frac{\eta_i}{{\phi_N^{\gamma_2}}^2(\eta_i)}, \quad i=0,1,\ldots,N\end{aligned} \tag{2.33}$$

are known as the Christofell numbers of the Laguerre-Gauss quadrature in terms of the normalized Laguerre polynomials [6]. Now, plugging (2.26) into (2.23) we obtain

$$\Phi(\xi_m,\eta_i) = (N+1)\sqrt{(N+\gamma_1+1)(N+\gamma_2+1)}\frac{\phi_N^{\gamma_1}(\xi_m)\phi_N^{\gamma_2}(\eta_i)}{\sqrt{\xi_m\eta_i}}. \tag{2.34}$$

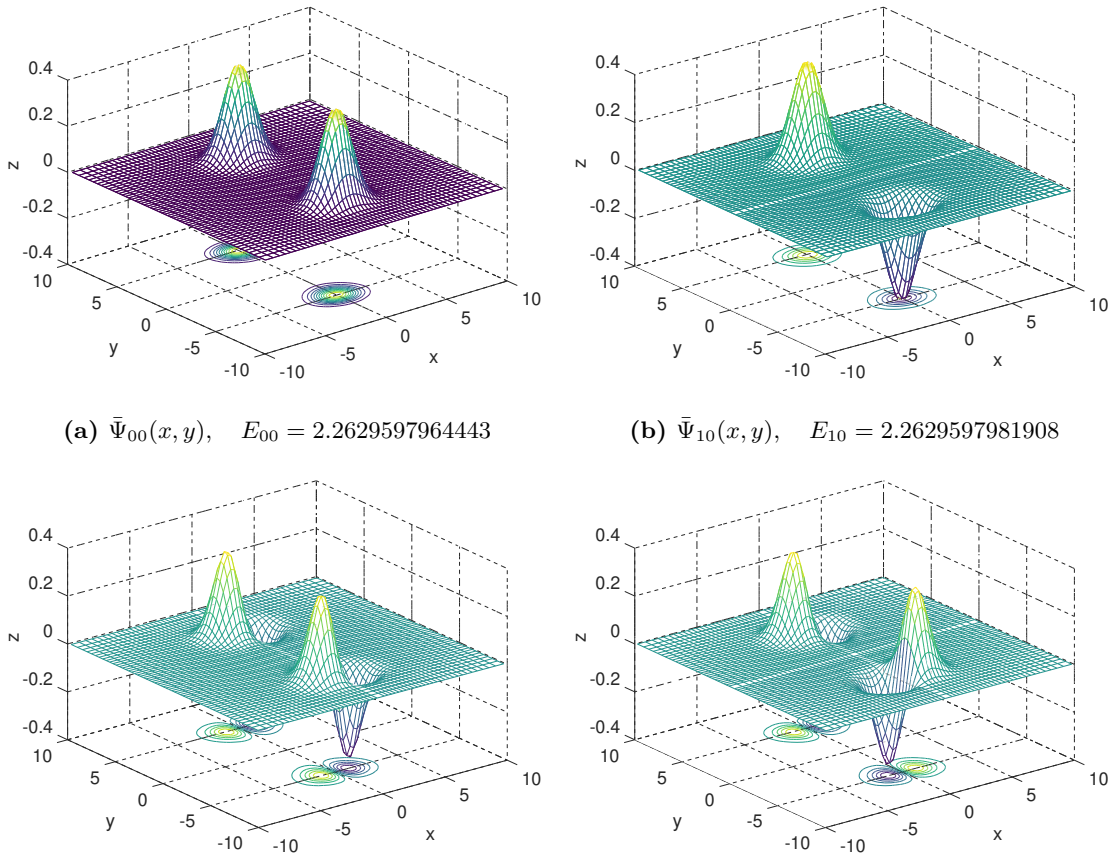
Finally, with the help of (2.34) and (2.33), (2.32) takes the form

$$\left\|\bar{\Psi}_k\right\|_{L^2}^2 = \lim_{N\to\infty}\sum_{n=0}^{N}\sum_{j=0}^{N}(u_{nj}^k)^2 \tag{2.35}$$

in which the term with double sum is the squared Euclidean 2-norm of the vector $\mathbf{u}^k_{(N+1)^2\times 1}$. Thus we have

$$\left\|\bar{\Psi}_k\right\|_{L^2}^2 = \lim_{N\to\infty}\left\|\mathbf{u}^k\right\|_2^2 = \lim_{N\to\infty}1 = 1 \tag{2.36}$$

since $\left\|\mathbf{u}^k\right\|_2 = 1$ by hypothesis which completes the proof. □



(a) $\bar{\Psi}_{00}(x,y)$, $E_{00} = 2.2629597964443$ **(b)** $\bar{\Psi}_{10}(x,y)$, $E_{10} = 2.2629597981908$

(c) $\bar{\Psi}_{01}(x,y)$, $E_{01} = 3.9992895301372$ **(d)** $\bar{\Psi}_{11}(x,y)$, $E_{11} = 3.9992895313331$

Figure 1. First four normalized wavefunctions of the symmetric double-well potential in (3.1) when $\mu = 0.01$.

3. Numerical results and discussion

In this section, we apply the methods described in the previous section to several symmetric two dimensional quantum mechanical potentials. As a first example we consider the symmetric double-well potential

$$V(x,y) = x^2 - y^2 + \mu y^2(2y^2 - x^2) + \frac{1}{8\mu} \tag{3.1}$$

where μ is a positive real parameter. In all tables, n stands for the eigenvalue index, N the truncation order for which the desired accuracy of the corresponding eigenvalue is obtained, and α_{opt} denotes the optimum value of the scaling or an optimization parameter α for which the desired accuracy is obtained with the smallest possible truncation order N. A method to determine the optimum value of α for Gaussian type functions is given in [10] which can also be applied in our problem since the eigenfunctions of (1.1) are of Gaussian type.

The accuracy of the results in all tables reported here has been checked by inspecting the number of stable digits between two consecutive truncation orders. Therefore, only the last digits might be incorrect because of rounding.

Table 1 presents the accuracy improvement of the ground state eigenvalue of the symmetric double well potential by systematically increasing the truncation size N. It is clear from Table 1 that the increase in N by one results in an accuracy gain of one digit for

Table 1. Accuracy improvement of the ground state eigenvalue of the symmetric double well potential in (3.1).

μ	α_{opt}	N	$E_{0,0}$
0.01	1	12	2.261
		15	2.262 956
		18	2.262 959 790
		21	2.262 959 796 46
		24	2.262 959 796 444 69
		27	2.262 959 796 444 740
		28	2.262 959 796 444 740

this potential. This is typical for all potentials considered here. In fact, for some specific potentials the accuracy gain is more than one digit when the truncation size is increased by one.

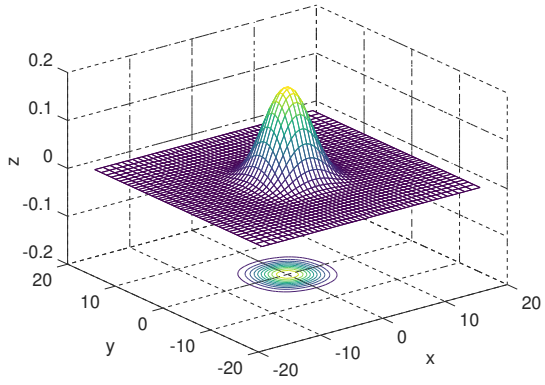
Table 2. Several nearly degenerate eigenvalues of the symmetric double-well potential in (3.1). For comparison, we include the corresponding results from [1] which uses the HPM. For both methods $\alpha_{opt} = 1$.

μ	N_{LPM}	N_{HPM}	$E_{2m,2n}$ LPM/HPM	$E_{2m,2n+1}$ LPM/HPM
0.01	28	56	2.262 959 796 444 3 / 43	2.262 959 798 190 7 / 08
			4.967 130 049 336 0 / 68	4.967 130 461 753 9 / 38
			5.734 657 066 616 3 / 67	5.734 657 071 515 1 / 51
			7.523 965 294 560 8 / 11	7.524 006 494 536 1 / 68
			8.458 313 203 321 6 / 21	8.458 314 106 626 5 / 68
			9.203 671 170 577 8 / 78	9.203 671 208 017 7 / 80
			9.898 300 048 693 6 / 40	9.900 487 409 690 5 / 10
			11.045 853 380 364 7 / 47	11.045 937 822 097 3 / 73
			11.936 552 764 608 0 / 86	11.936 627 549 541 6 / 12
			11.994 455 823 810 8 / 09	12.054 502 192 145 4 / 51
			12.672 301 933 093 4 / 32	12.672 302 141 021 5 / 18
			$E_{2m+1,2n}$ LPM/HPM	$E_{2m+1,2n+1}$ LPM/HPM
			3.999 289 530 137 4 / 72	3.999 289 531 333 6 / 31
			6.714 422 914 369 3 / 92	6.714 423 198 940 9 / 15
			7.469 353 731 555 9 / 53	7.469 353 740 847 8 / 72
			9.287 707 580 307 3 / 73	9.287 736 596 968 9 / 88
			10.198 992 794 453 7 / 37	10.198 994 433 172 2 / 23
			10.937 895 736 016 2 / 57	10.937 895 835 513 0 / 31
			11.685 001 492 931 3 / 05	11.686 593 204 436 4 / 59

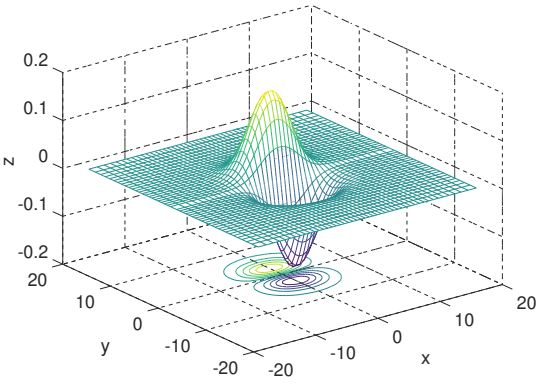
Table 2 presents some nearly degenerate states of the symmetric double-well potential. For comparison we include the results of [1], which uses Hermite pseudospectral methods in both direction. It is clear from Table 2 that the use of Laguerre instead of Hermite polynomials halved the truncation size in each direction that is necessary to obtain the accuracy quoted. More clearly, by using the HPM we need to diagonalize a matrix of size $(2N)^2 \times (2N)^2$ while with the use of LPM we only need to diagonalize four separate $N^2 \times N^2$ matrices to get the same number of eigenvalues to the same accuracy.

As a second example, we take into account the Gaussian type potential

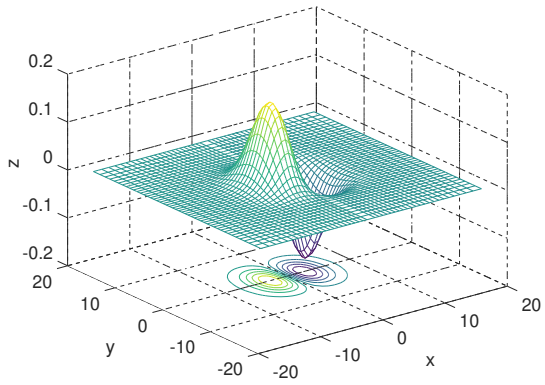
$$V(x, y) = -e^{-\beta(x^4+y^4)}, \qquad \beta > 0 \tag{3.2}$$



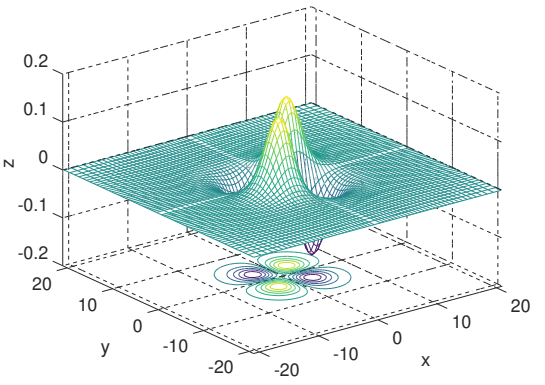
(a) $\bar{\Psi}_{00}(x,y)$, $E_{00} = -0.8002386220129$



(b) $\bar{\Psi}_{10}(x,y)$, $E_{10} = -0.5544027490889$



(c) $\bar{\Psi}_{01}(x,y)$, $E_{01} = -0.5544027490889$



(d) $\bar{\Psi}_{11}(x,y)$, $E_{11} = -0.3214069787951$

Figure 2. First four normalized wavefunctions of the Gaussian type potential in (3.2) when $\beta = 0.001$.

Table 3. Comparison of the truncation sizes of the LPM and HPM for the discrete states of the Gaussian potential in (3.2) when $\beta = 0.001$.

N_{LPM}	N_{HPM}	α_{opt}	$E_{2m,2n}$
30	60	0.5	-0.800 238 622 012 9
		0.3	-0.270 627 665 0
			-0.252 579 345 5
			$E_{2m,2n+1}$ and $E_{2m+1,2n}$
30	60	0.5	-0.554 402 749 088
		0.3	-0.064 141 040
		0.2	-0.004 59
			$E_{2m+1,2n+1}$
30	60	0.5	-0.321 406 978 7

which has a finite number of discrete states between $-1 < E_{m,n} < 0$ together with a continuous spectrum over the entire positive real axis for small values of the real parameter β.

Next, as a third example, we consider the hyperbolic secant potential

$$V(x,y) = -m(m+1)\,\mathrm{sech}^2\left[(x^4+y^4)^{1/2}\right] \tag{3.3}$$

Table 4. Improved results for the discrete states of the Gaussian potential in (3.2) when $\beta = 0.001$ by using LPM.

N_{LPM}	α_{opt}	$E_{2m,2n}$
42	0.5	-0.800 238 622 012 9
	0.3	-0.270 627 664 825 0
		-0.252 579 345 455 4
		$E_{2m,2n+1}$ and $E_{2m+1,2n}$
35	0.5	-0.554 402 749 088 9
48	0.3	-0.064 141 043 49
60	0.2	-0.004 589 7
		$E_{2m+1,2n+1}$
48	0.5	-0.321 406 978 795 1

where $m > 0$. Like the Gaussian potential, there exist finitely many discrete states located on the negative real axis between $-m(m+1) < E < 0$ together with the continuous spectrum on the whole positive real axis. Tables 3 and 5 presents the computed eigenvalues of the Gaussian type and hyperbolic secant potential by using the LPM and HPM.

Table 5. Comparison of the truncation sizes of the LPM and HPM for the discrete states of the hyperbolic secant potential in (3.3) when $m = 5$.

N_{LPM}	N_{HPM}	α_{opt}	$E_{2m,2n}$
30	60	2.5	-23.904 156 425 734
		2.0	-8.276 916 534 5
			-7.607 559 120 2
			$E_{2m,2n+1}$ and $E_{2m+1,2n}$
30	60	2.5	-16.505 099 700 87
		1.5	-2.343 009
			-0.532 94
			$E_{2m+1,2n+1}$
30	60	2.0	-9.599 644 620 3

For the last two potentials again we see that $N_{HPM} \approx 2N_{LPM} = 60$. Therefore, by increasing the truncation size N_{LPM} of the present algorithm it is possible to obtain more accurate results than the HPM which are presented in Tables 4 and 6. However, a remarkable slowing down of the convergence is met for the discrete states at the border of the continuum which is a common drawback of almost all methods even in the one-dimensional case. This is because of the nonexistence of the contributions coming from the continuous spectrum eigenfunctions in the basis functions [3, 11].

Finally, we take into account the quartic anharmonic oscillator

$$V(x,y) = x^2 + y^2 + c_4(x^4 + 2ax^2y^2 + y^4) \tag{3.4}$$

with $c_4 > 0$, and $-1 \le a \le 1$. Table 7 present the states $E_{2m,2n}$, $E_{2m,2n+1}$, $E_{2m+1,2n}$ and $E_{2m+1,2n+1}$ when $c_4 = 1000$ and $a = 1$. For comparison we also tabulate the results from [13] that employs the certain trigonometric basis set in a Rayleigh-Ritz variational scheme. We have executed our computer program in *gfortran–4.8* by using quadruple precision arithmetic so that the comparison of the numerical results with those of [13] becomes more meaningful and informative. Clearly, our results are slightly better than those of [13] where $17-18$ decimal points of accuracy was obtained with the truncation size of $N = 22$. On the other hand, with the same truncation size, we obtain $18 - 22$ decimal points of accuracy. Moreover, the algorithm of [1] is also implemented in Fortran programming language and

Table 6. Improved results for the discrete states of the hyperbolic secant potential in (3.3) when $m = 5$ by using LPM.

N_{LPM}	α_{opt}	$E_{2m,2n}$
30	2.5	-23.904 156 425 734
33	2.0	-8.276 916 534 56
		-7.607 559 120 19
		$E_{2m,2n+1}$ and $E_{2m+1,2n}$
30	2.5	-16.505 099 700 872 2
60	1.5	-2.343 009 097 47
		-0.532 963 25
		$E_{2m+1,2n+1}$
60	2.0	-9.599 644 620 311

executed in quadruple precision arithmetic. Again, the doubling $N_{HPM} \approx 2N_{LPM} = 44$ in the truncation sizes of the HPM and LPM is clear. Note that the HPM produces the full spectrum at once, however, while reporting in Table 7 we split it into four states to compare the results easily.

Table 7. First few energy eigenvalues of the quartic anharmonic oscillator in (3.4) when $c_4 = 1000$, $a = 1$.

N_{LPM}	N_{HPM}	$E_{2m,2n}$ $(\alpha_{opt} = 6)$ LPM $(N = 22)$/HPM $(N = 44)$	$E_{2m,2n}$ $(\alpha_{cr} = 1.5)$ Reference [13] $(N = 22)$
22	44	23.513 389 183 129 853 963 236 1	23.513 389 183 129 853 963
		89.433 434 033 749 367 276 85	89.433 434 033 749 367 277
		95.437 449 804 059 634 223 44	95.437 449 804 059 634 223
		170.997 778 280 937 441 267	170.997 778 280 937 441 27
		183.306 338 107 785 976 427	183.306 338 107 785 976 43
		187.549 037 142 026 458 968	187.549 037 142 026 458 97
		$E_{2m,2n+1}$ and $E_{2m+1,2n}$	$E_{2m,2n+1}$ and $E_{2m+1,2n}$
		54.054 855 795 519 439 394 244 4	54.054 855 795 519 439 394
		128.619 616 180 914 730 350 60	128.619 616 180 914 730 35
		138.283 038 429 442 399 890 09/11	138.283 038 429 442 399 89
		216.151 947 586 633 607 188 0/1	216.151 947 586 633 607 19
		$E_{2m+1,2n+1}$	$E_{2m+1,2n+1}$
		89.433 434 033 749 367 276 845 8	89.433 434 033 749 367 277
		170.997 778 280 937 441 267 36	170.997 778 280 937 441 27
		183.306 338 107 785 976 426 61	183.306 338 107 785 976 43

Closeness in the numerical results with the same truncation size is not too much surprising since both the trigonometric and Laguerre basis sets are somehow the exact solutions of the problem in (1.1). More specifically, the former is the exact solution of (1.1) over a finite rectangle $(x, y) \in (\alpha, \alpha) \times (\beta, \beta)$ with Dirichlet boundary conditions in which the potential is in the form of a rectangular box with impenetrable walls [13]. The latter is the solution of the system (1.1)-(1.2) under the two-dimensional harmonic oscillator potential $V(x, y) = x^2 + y^2$ (see the transformed equation (1.12) together with (1.13)-(1.14) when $\alpha = 1$).

4. Conclusion

In this article, the two-dimensional Schrödinger equation over the whole real plane with symmetric nonseparable potentials is solved numerically by using the LPM. Transformation of the problem over the first quadrant enabled us to treat the states $E_{2m,2n}$, $E_{2m,2n+1}$, $E_{2m+1,2n}$ and $E_{2m+1,2n+1}$ separately. By this way, instead of diagonalizing a matrix of size $4N^2 \times 4N^2$ we compute the eigenvalues of four matrices of size $N^2 \times N^2$ to obtain the same number of eigenvalues to a certain accuracy.

It is known that the numerical eigenvalue problems suffer from the problem of computing the full set of eigenvalues with a uniform accuracy [14]. Only the portion of the eigenvalues can be obtained with a desired accuracy for a fixed truncation order N. Therefore, the treatment of the states $E_{2m,2n}$, $E_{2m,2n+1}$, $E_{2m+1,2n}$ and $E_{2m+1,2n+1}$ by separate basis sets quadruples the number of high accurate eigenvalues for the same fixed truncation size N.

On the other hand, comparison of the present numerical results with those obtained by applying the HPM [1] reveals evidently that $N_{HPM} \approx 2N_{LPM}$. Clearly, the use of LPM instead of HPM halves the number of points and reduces the cost by a factor of two in each direction which strongly supports the main argument of the present study. Note that, we do not claim that the LPM is superior to the HPM from the efficiency or accuracy point of view in general. In fact, even the direct comparison of these two methods is not meaningful since the Hermite and Laguerre polynomials are defined over the whole real line and half line, respectively. However, here we have shown that if the system (1.1)-(1.2) has the reflection symmetries, that is, both the differential equation in (1.1) and the boundary conditions in (1.2) are invariant under the replacement of the independent variables x and/or y by their negatives, then the transformation of the problem over the first quadrant and the use of LPM with $\gamma = \pm\frac{1}{2}$ separate the states $E_{2m,2n}$, $E_{2m,2n+1}$, $E_{2m+1,2n}$ and $E_{2m+1,2n+1}$, and hence, halve the truncation size N in each direction. This reduction is important since in two dimension the size of the resulting discrete system increases as the square of the truncation size. Alternatively, without transforming the equation, one may use the even or odd indexed Hermite polynomials as basis sets to separate the above four states. Actually, both approaches can be regarded as equivalent if we remember the interrelations

$$H_{2n}(x) = (-1)^n 2^{2n} n! L_n^{-1/2}(x^2) \tag{4.1}$$

and

$$H_{2n+1}(x) = (-1)^n 2^{2n+1} n! x L_n^{1/2}(x^2) \tag{4.2}$$

between the Hermite and Laguerre polynomials. Unfortunately, direct use of $H_{2n}(\xi)$ or $H_{2n+1}(\xi)$ in (2.2) does not allow the separation of the above states. Thus, in this study we have presented the use of $L_n^{\gamma}(\xi)$ with $\gamma = \pm\frac{1}{2}$ after the transformation of the problem over the first quadrant in order to reduce the total cost by a factor of four. As a result, the same accuracy of the HPM for the numerical eigenvalues is obtained with considerably low cost which is in accordance with the main aim of this study. Remember that our claim was to present a pseudospectral method for the numerical solution of the two dimensional Schrödinger equation with *symmetric* nonseparable potentials which is more efficient than the HPM from a computational point of view.

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