*Journal of Mathematical Chemistry, Vol. 41, No. 4, May 2007 (© 2006)*
DOI: 10.1007/s10910-006-9083-z

# The Laguerre pseudospectral method for the reflection symmetric Hamiltonians on the real line

H. Taşeli* and H. Alıcı

*Department of Mathematics, Middle East Technical University, 06531 Ankara, Turkey*
E-mail: taseli@metu.edu.tr

Received 8 February 2006

Hermite–Weber functions provide a natural expansion basis for the numerical treatment of the Schrödinger equation on the whole real line. For the reflection symmetric Hamiltonians, however, it is shown here that the transformation of the problem over the half line and use of a Laguerre basis is computationally much more efficient in a pseudospectral scheme.

**KEY WORDS:** Schrödinger operator, quantum mechanical oscillators, singular Sturm–Liouville problems on the real line, spectral and pseudospectral methods, Laguerre polynomials, Laguerre collocation points

**AMS subject classification:** 65L60, 81Q05, 65L15, 34L40, 42C10

## 1. Introduction

This is the third in a series of papers dealing with the numerical solutions of the singular Sturm–Liouville eigenvalue problems, described by the Hamiltonian

$$\mathcal{H} = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x), \quad x \in (-\infty, \infty) \tag{1}$$

by means of a spectral method. In recent articles [1] and [2] (hereafter referred to as PI and PII, respectively), Taşeli and Erseçen and Taşeli and Alıcı presented the continuous (spectral, Rayleigh–Ritz) and discrete (pseudospectral, collocation) variable representations of the scaled Hermite–Weber basis, respectively, applied to the problem being considered with several non-singular quantum mechanical potentials $V(x)$.

In PI and PII, we consequently deduced that the convergence rates of the Rayleigh–Ritz and pseudospectral methods based on the normalized Hermite–Weber functions were almost the same except for the reflection symmetric potentials, where $V(x) = V(-x)$. For a reflection symmetric Hamiltonian, the

*Corresponding author.

potential may be regarded as a function of $x^2$, i.e., $v(x^2) := V(x)$, and hence the spectrum can be decomposed into two disjoint subsets containing solely the even and odd eigen-levels, respectively. In general, however, the nature of the Lagrange interpolant in a pseudospectral scheme, particularly in the Hermite pseudospectral method (HPM) suggested by PII, is not suitable for an independent treatment of the even and odd parity wavefunctions. For this reason, we reported a doubling in the truncated matrix sizes in PII compared with those of PI, when the calculation of the eigenvalues of symmetric potentials within the same accuracy is required.

Therefore, the main aim of this paper is to introduce a pseudospectral method for potentials of the form $V(x) = v(x^2)$ over $x \in (-\infty, \infty)$ in which trial solutions to the even and odd eigenfunctions can be proposed separately. First of all the symmetry of the potential function suggests the use of a quadratic transformation

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

which converts the Schrödinger equation $\mathcal{H}\Psi = E\Psi$ to the form

$$\left[\xi \frac{\mathrm{d}^2}{\mathrm{d}\xi^2} + \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}\xi} - \frac{1}{4\alpha^2} v(\xi/\alpha^2)\right] \Psi(\xi) = -\frac{E}{4\alpha^2}\Psi(\xi), \quad \xi \in (0, \infty), \tag{3}$$

where $\alpha$ is an optimization parameter. Clearly, the Hermite–Weber functions in PI and PII provide an orthonormal basis over the whole real line whereas the transformed equation (3) is defined on the half line. Thus the HPM of PII is not preferable anymore. Alternatively, it seems that an appropriate Laguerre basis $\{L_n^\gamma(\xi)\}_{n=0,1,\ldots}$, in which the $L_n^\gamma$ denote the Laguerre polynomials (sometimes the $L_n^\gamma$ are known more precisely as the generalized or associated Laguerre polynomials of degree $n$ and order $\gamma$), may be used by recalling the fact that it is an orthogonal set on $(0, \infty)$ with respect to the weighting function $\xi^\gamma \mathrm{e}^{-\xi}$ for $\gamma > -1$.

Hence, section 2 is concerned with the pseudospectral formulation of the computational problem corresponding to the transformed Schrödinger equation (3) by means of a Laguerre basis. In the last section we present a number of computer experiments and discuss the results.

## 2. The Laguerre pseudospectral method (LPM)

Let us start with a solution of the type

$$\Psi(\xi) = \xi^p \, \mathrm{e}^{-\xi/2} y(\xi), \quad p \in \mathbb{R} \tag{4}$$

satisfying the asymptotic boundary condition at infinity, where the factor $\xi^p$ has been introduced to cope with the *artificial* singularity of (3) at $\xi=0$. Note that the original Hamiltonian (1) is in fact regular everywhere except the "point at infinity", and the additional singularity of (3) at the origin has been resulted from using the quadratic transformation (2). Substitution of (4) into (3) leads to the equation that the new dependent variable $y(\xi)$ must satisfy

$$\xi y'' + (2p + \tfrac{1}{2} - \xi)y' + \frac{1}{4\alpha^2}\left[\alpha^2\xi - v(\xi/\alpha^2) + 2p(2p-1)\frac{\alpha^2}{\xi}\right]y = \frac{1}{4\alpha^2}\big[(4p+1)\alpha^2 - E\big]y \tag{5}$$

implying that the unwelcome singularity located at the origin can be removed if $p$ is either 0 or 1/2. Therefore, setting

$$2p + \tfrac{1}{2} = \gamma + 1 \tag{6}$$

we then express (5) in the more neatly form

$$\xi y'' + (\gamma + 1 - \xi)y' + q(\xi;\alpha)y = \mathcal{E}(\alpha,\gamma)y, \quad \xi \in (0,\infty) \tag{7}$$

with $\gamma = \mp 1/2$, where

$$q(\xi;\alpha) := \frac{1}{4\alpha^2}\big[\alpha^2\xi - v(\xi/\alpha^2)\big] \tag{8}$$

and

$$\mathcal{E}(\alpha,\gamma) := \frac{1}{4\alpha^2}\big[2(\gamma+1)\alpha^2 - E\big] \tag{9}$$

denote the modified potential and eigenvalue parameter, respectively.

Now it is clear that the solutions in (4) with $p = 0$ ($\gamma = -1/2$) and $p = 1/2$ ($\gamma = 1/2$) yield even and odd eigenfunctions, respectively, on returning back to the original variable $x$ via (2). Accordingly, as we expected, the new setup of the problem in (7) allows us to determine symmetric and antisymmetric states separately, for the two specific parameter values of $\gamma = -1/2$ and $\gamma = 1/2$. Furthermore, (7) is much akin to the differential equation

$$\xi y'' + (\gamma + 1 - \xi)y' = -ny, \quad n = 0, 1, \ldots \tag{10}$$

of the Laguerre polynomials $L_n^{\gamma}(\xi)$, especially, when $q(\xi;\alpha)$ is viewed as a perturbation over the *zero* potential.

In the traditional Rayleigh–Ritz method, one may propose a trial solution of the form

$$y_{\mathrm{T}}(\xi) = \sum_{n=0}^{N} c_n \psi_n(\xi) \tag{11}$$

i.e., a truncated eigenfunction expansion in terms of the normalized Laguerre polynomials

$$\psi_n(\xi) = \sqrt{n!/\Gamma(\gamma+n+1)}\, L_n^{\gamma}(\xi) \tag{12}$$

substitute into (7), and multiply both sides by $\psi_m(\xi)$ in order to arrive at the algebraic system $\mathcal{A}\boldsymbol{c} = \mathcal{E}\boldsymbol{c}$ with the matrix elements

$$\mathcal{A}_{mn} = -n\delta_{mn} + Q_{mn}, \quad Q_{mn} = \int_0^{\infty} q(\xi)\xi^{\gamma}\mathrm{e}^{-\xi}\psi_m(\xi)\psi_n(\xi)\mathrm{d}\xi \tag{13}$$

upon performing inner products relative to the weight $\xi^{\gamma}\mathrm{e}^{-\xi}$ over $\xi \in (0,\infty)$, where $\delta_{mn}$ is the Kronecker's delta. Obviously, the constants $c_n$ represent the Fourier coefficients in the continuous expansion of $y(\xi)$, which is actually a polynomial of degree $N$.

On the other hand, a pseudospectral method is based on choosing $N+1$ nodes or collocation points, say $\xi_0, \xi_1, \ldots, \xi_N$, and then using the actual values of $y(\xi)$, that is, $y_0 = y(\xi_0)$, $y_1 = y(\xi_1)$, $\ldots$, $y_N = y(\xi_N)$, at the specified nodes to construct an interpolation polynomial of degree $N$

$$y_{\mathrm{T}}(\xi) = \sum_{n=0}^{N} y_n \ell_n(\xi) \tag{14}$$

by means of the Lagrange formula [3], which suggests another polynomial approximation to a typical solution of (7). Such a pseudospectral scheme in which the $N$th degree Lagrange polynomials $\ell_n(\xi)$ are defined by the normalized or standard Laguerre polynomials

$$\ell_n(\xi) = \frac{\psi_{N+1}(\xi)}{(\xi-\xi_n)\psi'_{N+1}(\xi_n)} = \frac{L_{N+1}^{\gamma}(\xi)}{(\xi-\xi_n)\Big[\dfrac{\mathrm{d}}{\mathrm{d}\xi}L_{N+1}^{\gamma}(\xi)\Big]_{\xi=\xi_n}}, \quad n = 0, 1, \ldots, N \tag{15}$$

is called a LPM, where the nodes $\xi_n$ are the real, distinct and positive roots of $L_{N+1}^{\gamma}(\xi)$. Here, recall the key property of the Lagrange polynomials that $\ell_n(\xi_m) = \delta_{mn}$ for all $m$ and $n$. In this article, the discretization procedure of (7) by the LPM in its full generality, for any arbitrary $\gamma$ parameter, is presented keeping in mind that we will eventually take $\gamma = \mp 1/2$ to approximate the even and odd solutions of the original reflection symmetric system.

First we need to fix the nodal points $\xi_n$ accurately. Employing the well-known relation

$$(n+1)L_{n+1}^{\gamma}(\xi) = (2n+\gamma+1-\xi)L_n^{\gamma}(\xi) - (n+\gamma)L_{n-1}^{\gamma}(\xi)$$

we find the three-term recursion

$$\sqrt{n(n+\gamma)}\psi_{n-1}(\xi) - (2n+\gamma+1-\xi)\psi_n(\xi) + \sqrt{(n+1)(n+\gamma+1)}\psi_{n+1}(\xi) = 0 \tag{16}$$

for the normalized Laguerre polynomials and consider its first $N+1$ equations, provided by $n = 0, 1, \ldots, N$, to write the inhomogeneous linear system

$$(\xi \boldsymbol{I} - \boldsymbol{R})\boldsymbol{x} = \boldsymbol{b}, \tag{17}$$

where $\boldsymbol{R}$ is the tridiagonal symmetric matrix

$$\boldsymbol{R} = \begin{bmatrix} \gamma+1 & -\sqrt{\gamma+1} & 0 & \cdots & 0 \\ -\sqrt{\gamma+1} & \gamma+3 & -\sqrt{2(\gamma+2)} & \ddots & \vdots \\ 0 & -\sqrt{2(\gamma+2)} & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \gamma+2N-1 & -\sqrt{N(\gamma+N)} \\ 0 & \cdots & 0 & -\sqrt{N(\gamma+N)} & \gamma+2N+1 \end{bmatrix} \tag{18}$$

of dimension $(N+1)\times(N+1)$, $\boldsymbol{b}$ the $(N+1)-$vector

$$\boldsymbol{b} = \left[0, 0, \ldots, 0, \sqrt{(N+1)(N+\gamma+1)}\ \psi_{N+1}(\xi)\right]^{\mathrm{T}} \tag{19}$$

with only one non-zero component, and $\boldsymbol{I}$ the identity matrix. To determine the nodes, we require that $\psi_{N+1}(\xi) = 0$ and notice that the system (17) reduces to the standard matrix eigenvalue problem $\boldsymbol{R}\boldsymbol{x} = \xi\boldsymbol{x}$. Hence the first $N+1$ roots $\xi_n$ of the Laguerre polynomials appear to be the eigenvalues of the matrix $\boldsymbol{R}$.

Then we put the interpolant (14) into (7)

$$\sum_{n=0}^{N}\left[\xi\ell_n''(\xi) + (\gamma+1-\xi)\ell_n'(\xi) + q(\xi;\alpha)\ell_n(\xi)\right]y_n = \mathcal{E}(\alpha,\gamma)\sum_{n=0}^{N}\ell_n(\xi)y_n \tag{20}$$

and demand its satisfaction at the grid points $\xi_m$ for $m = 0, 1, \ldots, N$, leading to the discrete representation

$$\widehat{\boldsymbol{\mathcal{B}}}\boldsymbol{y} = \mathcal{E}(\alpha,\gamma)\boldsymbol{y} \tag{21}$$

of our differential equation for the computation of an eigenvector $\boldsymbol{y} = [y_0, y_1, \ldots, y_N]^{\mathrm{T}}$ corresponding to a modified eigenvalue $\mathcal{E}$. Here, the general entry $\widehat{B}_{mn}$ of $\widehat{\boldsymbol{\mathcal{B}}}$ has the form

$$\widehat{B}_{mn} = \widehat{K}_{mn} + q_m\delta_{mn}, \quad m, n = 0, 1, \ldots, N \tag{22}$$

in which $q_m := q(\xi_m;\alpha)$ stands for the diagonal potential matrix and $\widehat{K}_{mn}$ the kinetic energy term that is expressible as

$$\widehat{K}_{mn} = \xi_m d^{(2)}_{mn} + (\gamma + 1 - \xi_m) d^{(1)}_{mn} \tag{23}$$

in terms of the so-called differentiation matrices $d^{(1)}_{mn} = \ell'_n(\xi_m)$ and $d^{(2)}_{mn} = \ell''_n(\xi_m)$ (see equations 16 and 19 of PII for details). More specifically, making use of the differential-difference relation

$$\xi \frac{\mathrm{d}}{\mathrm{d}\xi} L^{\gamma}_n(\xi) = n L^{\gamma}_n(\xi) - (n+\gamma) L^{\gamma}_{n-1}(\xi) \;\Rightarrow\; \xi \psi'_n(\xi) = n\psi_n(\xi) - \sqrt{n(n+\gamma)}\,\psi_{n-1}(\xi) \tag{24}$$

and the differential equation (10), we obtain

$$d^{(1)}_{mn} = \frac{1}{2} \begin{cases} \dfrac{2}{\xi_m - \xi_n} \dfrac{\xi_n \psi_N(\xi_m)}{\xi_m \psi_N(\xi_n)} & \text{if } m \neq n \\ \dfrac{1}{\xi_n}(\xi_n - \gamma - 1) & \text{if } m = n \end{cases} \tag{25}$$

and

$$d^{(2)}_{mn} = \frac{1}{3} \begin{cases} \dfrac{3}{\xi_m - \xi_n} \left[ \dfrac{1}{\xi_m}(\xi_m - \gamma - 1) - \dfrac{2}{\xi_m - \xi_n} \right] \dfrac{\xi_n \psi_N(\xi_m)}{\xi_m \psi_N(\xi_n)} & \text{if } m \neq n \\ \dfrac{1}{\xi_n} \left[ \dfrac{1}{\xi_n}(\xi_n - \gamma - 1)(\xi_n - \gamma - 2) - N \right] & \text{if } m = n. \end{cases} \tag{26}$$

explicitly. Nevertheless, as stated in PII, it is again more amenable to consider the total kinetic energy matrix given by (23), the derivation of which can be accomplished after some algebra,

$$\widehat{K}_{mn} = -\frac{1}{6} \begin{cases} \dfrac{12\xi_n}{(\xi_m - \xi_n)^2} \dfrac{\psi_N(\xi_m)}{\psi_N(\xi_n)} & \text{if } m \neq n \\ 2N + \dfrac{1}{\xi_n}\left[(\gamma - \xi_n)^2 - 1\right] & \text{if } m = n \end{cases} \tag{27}$$

by exploiting the functional identities such as (10), (16) and (24) available for the Laguerre polynomials. Clearly $\widehat{K}_{mn} \neq \widehat{K}_{nm}$, however, its simple structure suggests immediately introducing a similarity transformation

$$\boldsymbol{\mathcal{B}} = \boldsymbol{P}^{-1} \widehat{\boldsymbol{\mathcal{B}}} \boldsymbol{P} \tag{28}$$

to replace the coefficient matrix of (21) with a symmetric one. Actually, if $\boldsymbol{P}$ is chosen as a diagonal matrix of the form

$$\boldsymbol{P} = \mathrm{diag}\left[ \frac{\psi_{N,0}}{\sqrt{\xi_0}}, \frac{\psi_{N,1}}{\sqrt{\xi_1}}, \ldots, \frac{\psi_{N,m}}{\sqrt{\xi_m}}, \ldots, \frac{\psi_{N,N}}{\sqrt{\xi_N}} \right], \quad \psi_{N,m} = \psi_N(\xi_m) \tag{29}$$

then the matrix $\mathcal{B}$ can be defined by

$$B_{mn} = K_{mn} + q_m \delta_{mn}, \tag{30}$$

which is symmetric, since $K_{mn}$ reduces to

$$K_{mn} = -\frac{1}{6}\begin{cases} \dfrac{12\sqrt{\xi_m \xi_n}}{(\xi_m - \xi_n)^2} & \text{if } m \neq n \\ 2N + \dfrac{1}{\xi_n}\left[(\gamma - \xi_n)^2 - 1\right] & \text{if } m = n \end{cases} \tag{31}$$

with $K_{mn} = K_{nm}$. Besides their simplicity, the symmetric matrix elements now depend only on the grid points $\xi_k$ and do not require any evaluation of the Laguerre polynomials. Hence, instead of the system (21), we may consider the symmetric matrix eigenvalue problem

$$\mathcal{B}\boldsymbol{u} = \mathcal{E}(\alpha, \gamma)\boldsymbol{u} \tag{32}$$

because the similar matrices share the same eigenvalue spectrum. Also, the connection formula

$$\boldsymbol{y} = \boldsymbol{P}\boldsymbol{u} \tag{33}$$

serves to return back to an eigenvector $\boldsymbol{y}$ of the non-symmetric system (21), by the help of a calculated eigenvector $\boldsymbol{u}$ of the symmetric matrix.

## 3. Numerical experiments and conclusion

The spectral and pseudospectral formulations in section 2 are applied to a class of symmetric potentials by making use of the Laguerre bases with $\gamma = -1/2$ and $\gamma = 1/2$. Specifically, we consider the test problems provided by the generalized anharmonic oscillators

$$V(x) = x^2 + v_{2k}x^{2k}, \quad v_{2k} > 0 \tag{34}$$

for $k = 2$ and 3, the symmetric double well potential (SDWP)

$$V(x) = v_4\left(x^2 - \tfrac{1}{2}v_4^{-1}\right)^2, \quad v_4 > 0 \tag{35}$$

and the non-polynomial Gaussian potential (GP)

$$V(x) = -e^{-\beta x^2}, \quad \beta > 0 \tag{36}$$

whose very well-known spectral properties can be found in the literature [4–7].

Typical computations for the ground state eigenvalues of the quartic and sextic oscillators as a function of the coupling constants $v_4$ and $v_6$ are displayed in tables 1 and 2, respectively. In all tables, $N_{\mathrm{RR}}$, $N_{\mathrm{HPM}}$ and $N_{\mathrm{LPM}}$

Table 1
Ground state energies of the quartic oscillator $V(x) = x^2 + v_4 x^4$, as a function of $v_4$.

| $v_4$ | $E_0$ | $N_{\mathrm{RR}}$ | $N_{\mathrm{HPM}}$ | $N_{\mathrm{LPM}}$ | $\alpha_{\mathrm{opt}}$ |
|---|---|---|---|---|---|
| $10^{-4}$ | 1.000 074 986 880 200 111 122 834 155 30 | 8 | 15 | 8 | 1 |
| $10^{-2}$ | 1.007 373 672 081 382 460 533 843 905 98 | 17 | 32 | 17 | 1 |
| 1 | 1.392 351 641 530 291 855 657 507 876 61 | 25 | 51 | 25 | 2.1 |
| 10 | 2.449 174 072 118 386 918 268 793 906 19 | 26 | 53 | 27 | 3.1 |
| $10^3$ | 10.639 788 711 328 046 063 622 042 669 4 | 30 | 56 | 27 | 6.5 |
| $10^4$ | 22.861 608 870 272 468 891 759 867 963 5 | 30 | 56 | 28 | 10 |
| $10^5$ | 49.225 447 584 229 625 157 076 387 001 1 | 30 | 56 | 28 | 14 |

Table 2
Ground state energies of the sextic oscillator $V(x) = x^2 + v_6 x^6$, as a function of $v_6$.

| $v_6$ | $E_0$ | $N_{\mathrm{RR}}$ | $N_{\mathrm{HPM}}$ | $N_{\mathrm{LPM}}$ | $\alpha_{\mathrm{opt}}$ |
|---|---|---|---|---|---|
| $10^{-4}$ | 1.000 187 228 153 680 768 286 355 665 62 | 16 | 30 | 16 | 1 |
| $10^{-2}$ | 1.016 741 363 754 732 031 671 817 981 51 | 32 | 70 | 34 | 1.8 |
| 1 | 1.435 624 619 003 392 315 761 272 220 54 | 39 | 78 | 39 | 3.2 |
| 10 | 2.205 723 269 595 632 351 009 973 387 17 | 40 | 78 | 40 | 4.2 |
| $10^3$ | 6.492 350 132 329 671 550 549 557 845 34 | 40 | 80 | 42 | 7.0 |
| $10^4$ | 11.478 798 042 264 543 961 289 816 038 6 | 39 | 78 | 40 | 9.5 |
| $10^5$ | 20.375 098 656 309 660 844 567 287 513 5 | 41 | 81 | 41 | 12 |

denote matrix sizes of the Rayleigh–Ritz, Hermite and Laguerre pseudospectral schemes, respectively, at which the desired accuracy is obtained.

Table 3 exhibits the nearly degenerate states of a SDWP for $v_4 = 0.01$, in which the two wells located symmetrically about the origin are sufficiently separated.

As a last example, a few even-indexed eigenvalues of the GP (36) have been presented in table 4. The GP has both continuous and a finite number of discrete eigenvalues lying between $-1 < E < 0$. It is known that there exists a threshold value $\beta_{\mathrm{thr}}$ for the parameter $\beta$ beyond which the particular bound state being considered can no longer survive. It can be seen from table 4 that, as in the other methods, a remarkable slowing down of convergence occurs for very weakly bound states with $E$ just below zero, when $\beta$ approaches $\beta_{\mathrm{thr}}$.

It should be noted that the continuous Rayleigh–Ritz treatment of the problem via Laguerre bases is equivalent to that of PI, where the sets of Hermite polynomials $\{H_{2n}\}$ and $\{H_{2n+1}\}$ were used separately for the approximations of symmetric and antisymmetric state wavefunctions. In fact, if we recall the interrelations [8]

$$H_{2n}(x) = (-1)^n 2^{2n} n! L_n^{-1/2}(x^2) \tag{37}$$

Table 3
Nearly degenerate states of the SDWP, $V(x) = v_4\left(x^2 - \frac{1}{2}v_4^{-1}\right)^2$ for $v_4 = 0.01$.

| $n$ | $E_n$ | $N_{\mathrm{RR}}$ | $N_{\mathrm{HPM}}$ | $N_{\mathrm{LPM}}$ | $\alpha_{\mathrm{opt}}$ |
|---|---|---|---|---|---|
| 0 | 1.404 048 605 297 706 882 425 707 570 82 | 52 | 104 | 52 | 1.0 |
| 1 | 1.404 048 605 297 706 882 602 566 280 56 | 52 | 104 | 52 | 1.0 |
| 2 | 4.170 193 605 999 310 127 833 875 071 30 | 54 | 108 | 54 | 1.0 |
| 3 | 4.170 193 605 999 310 219 613 291 198 73 | 54 | 108 | 54 | 1.0 |
| 4 | 6.870 088 833 714 024 612 172 315 168 49 | 56 | 112 | 56 | 1.0 |
| 5 | 6.870 088 833 714 046 802 425 995 681 89 | 56 | 112 | 56 | 1.0 |
| 6 | 9.489 578 387 187 870 055 194 418 356 55 | 58 | 116 | 58 | 1.0 |
| 7 | 9.498 578 387 191 178 212 320 856 961 14 | 58 | 116 | 58 | 1.0 |
| 8 | 12.049 309 486 334 092 592 332 880 171 6 | 59 | 118 | 59 | 1.1 |
| 9 | 12.049 309 486 673 006 847 573 312 477 9 | 59 | 118 | 59 | 1.1 |
| 10 | 14.514 205 022 981 239 103 429 421 443 9 | 60 | 120 | 60 | 1.1 |
| 11 | 14.514 205 048 121 017 338 991 612 415 8 | 60 | 120 | 60 | 1.1 |

Table 4
Eigenvalues of the GP $V(x) = -\mathrm{e}^{-\beta x^2}$, as a function of $\beta$.

| $\beta$ | $\alpha_{\mathrm{opt}}$ | $N_{\mathrm{RR}}$ | $N_{\mathrm{HPM}}$ | $N_{\mathrm{LPM}}$ | $n$ | $E_n$ |
|---|---|---|---|---|---|---|
| $10^{-3}$ | 0.2 | 30 | 56 | 28 | 0 | −0.968 752 703 034 398 668 606 599 656 91 |
| | | 35 | 70 | 35 | 2 | −0.846 820 196 725 804 118 603 225 951 44 |
| | | 45 | 85 | 43 | 4 | −0.731 125 549 125 734 739 132 375 767 29 |
| | | 55 | 103 | 52 | 6 | −0.621 888 650 443 182 657 155 148 987 66 |
| $10^{-2}$ | 0.3 | 41 | 81 | 41 | 0 | −0.903 763 987 980 773 054 539 687 567 95 |
| | | 70 | 128 | 69 | 2 | −0.550 801 670 798 557 886 254 842 935 81 |
| | | 70 | 128 | 69 | 4 | −0.267 463 693 629 351 027 |
| | | 70 | 128 | 69 | 6 | −0.068 692 251 |
| $10^{-1}$ | 0.2 | 70 | 148 | 74 | 0 | −0.721 530 628 487 107 638 685 036 884 81 |
| | | 70 | 148 | 74 | 2 | −0.007 90 |

and

$$H_{2n+1}(x) = (-1)^n 2^{2n+1} n! x L_n^{1/2}(x^2) \tag{38}$$

between the Hermite and Laguerre polynomials then it is not difficult to verify that the variational matrices in (13) are nothing but those in PI. However, the HPM of PII and the LPM of the present article stand for alternative numerical procedures of the problem. Evidently, we deduce from the numerical tables that $N_{\mathrm{HPM}} \approx 2N_{\mathrm{LPM}}$. Therefore, the most efficient pseudospectral discretization of the Schrödinger equation over $(-\infty, \infty)$ having a symmetric potential is not the HPM, and it is suggested by the LPM, which supports the main argument

of this paper. On the other hand, we see that $N_{\mathrm{LPM}} \approx N_{\mathrm{RR}}$ because both Rayleigh–Ritz and LPM take care of the symmetry of the potential.

Finally, the LPM which is considered here only for specific values of $\gamma = \pm 1/2$ might be much more generally applicable, for instance, to radial Schrödinger operators as well, where the radial variable is already defined on the half line $(0, \infty)$ naturally.

## Acknowledgment

This research was supported by a grant from TÜBİTAK, the Scientific and Technical Research Council of Turkey.

## References

[1] H. Taşeli and M.B. Erseçen, J. Math. Chem. 34 (2003) 177.
[2] H. Taşeli and H. Alıcı, J. Math. Chem. 38 (2005) 367.
[3] D. Funaro, *Polynomial Approximations of Differential Equations* (Springer-Verlag, Berlin, 1992).
[4] K. Banerjee and S.P. Bhatnagar, Phys. Rev. D 18 (1978) 4767.
[5] N. Bessis, G. Bessis and B. Joulakian, J. Phys. A 15 (1982) 3679.
[6] C.S. Lai, J. Phys. A 16 (1983) L181.
[7] M. Cohen, J. Phys. A 17 (1984) L101.
[8] M. Abramowitz and I.A. Stegun, *Handbook of Mathematical Functions* (Dover, New York, 1970) p. 779.