The Schrödinger equation on a Lagrange mesh

Gaotsiwe J Rampho

Department of Physics, University of South Africa, P.O. Box 392, Pretoria 0003, South Africa

E-mail: ramphjg@unisa.ac.za

Abstract. In this paper the Lagrange-mesh method is used to solve the two- and three-dimensional Schrödinger equation in spherical coordinates. Matrix elements that involve few free parameters and depend on the grid points for the Hamiltonian, and can be used with any quantum mechanical system, are employed. The accuracy of the matrix elements is tested with the quartic anharmonic oscillator and a double ring-shaped harmonic oscillator potentials. Eigenvalues for the systems are reproduced to within machine accuracy when the free parameters of the matrix elements are chosen appropriately.

1. Introduction

Atomic, molecular and nuclear systems are quantum mechanical systems that are accurately described by the Schrödinger equation. Theoretical studies of these systems are based on the solution to the many-body Schrödinger equation for the systems. However, the Schrödinger equation can be solve exactly only for a few types of potentials describing interactions in quantum systems [1, 2]. As a result, only numerical solutions of the equation with potentials of a general form are possible, even for systems with few constituents. A number of numerical methods is available to generate accurate numerical solutions to the Schrödinger equation [3, 4, 5, 6, 7, 8]. Except for the Lagrange-mesh method [8], many of the methods are computationally demanding and suffer from slow convergence. The Lagrange-mesh method is a variational method that employs specialized basis functions on a specialized grid to construct variational solutions for quantum dynamical equations. The method was shown to converge rapidly and generated simple and accurate numerical solutions for different quantum mechanical systems [9, 10, 11]. In the present work the Lagrange-mesh method is used to construct accurate numerical solutions to the two- and three-dimensional Schrödinger equation in polar coordinates. Not many instructive implementation of the method in polar coordinates, without the use of the spherical harmonics, are available.

The Lagrange-mesh method combines the variational technique through the Lagrange basis expansion with the collocation technique through quadrature rules to construct numerical solutions to quantum mechanical dynamical equations [8]. The method generates matrix elements, for the equations, that depend only on the collocation abscissas, resulting in a set of algebraic equations for the variational parameters that can be solved efficiently and accurately. The use of the Lagrange-mesh method in solving the multi-dimensional Schrödinger equation in polar coordinates has, so far, been generally restricted to the constant-mesh Lagrange functions [12] and the Lagrange-Legendre functions [8]. Matrix elements for the more general Lagrange-Jacobi mesh, from which the matrix elements for the Legendre mesh and other meshes can be obtained, are derived in [13]. This work discusses the specialization of the Lagrange-Jacobi

functions [13] to treat the angular components of the solution to the Schrödinger equation in polar coordinates.

This paper is organized as follows. The Schrödinger equation in two- and three-dimensions in spherical polar coordinates is presented in section 2. In section 3 the Lagrange meshes and Lagrange functions applicable to the three-dimensional Schrödinger equation in spherical polar coordinates are discussed. Matrix elements for the Hamiltonian of the equation are also developed. The simplicity and accuracy of the method is demonstrated by solving the Schrödinger equation for the two-dimensional quartic anharmonic oscillator potential as well as for the double ring-shaped harmonic oscillator potential. The results are discussed in section 4 and conclusions are given in section 5.

2. The Schrödinger equation

The configuration-space Schrödinger equation ($\hbar = 2m = 1$) in the two-dimensional cylindrical polar coordinates $\vec{r}(r, \phi)$ can be cast in the form

$$\left[-\frac{\partial^2}{\partial r^2} - \frac{1}{r^2} \left(\frac{\partial^2}{\partial \phi^2} + \frac{1}{4} \right) + V(r, \phi) \right] \Phi(r, \phi) = E\, \Phi(r, \phi) \tag{1}$$

where E denotes the energy, $\Phi(\vec{r})$ the reduced wave function and $V(\vec{r})$ the potential function. In the three-dimensional spherical coordinates $\vec{r}(r, \theta, \phi)$ the equation can be written in the form

$$\left\{ -\frac{\partial^2}{\partial r^2} - \frac{1}{r^2} \left[\frac{\partial^2}{\partial \theta^2} + \frac{1}{\sin^2 \theta} \left(\frac{\partial^2}{\partial \phi^2} + \frac{1}{4} \right) + \frac{1}{4} \right] + V(r, \theta, \phi) \right\} \Phi(r, \theta, \phi) = E\, \Phi(r, \theta, \phi) \tag{2}$$

where $r \in [0, \infty]$, $\theta \in [0, \pi]$ and $\phi \in [0, 2\pi]$. The square-integrable solutions $\Phi(\vec{r})$ to the equations are constructed with Dirichlet boundary conditions. A more general discussion of the Schrödinger equation in a D-dimensional spherical coordinate system will be given elsewhere.

In the Lagrange-mesh method the angular domains $(\theta, \phi) \in [0, \pi] \times [0, 2\pi]$ are mapped onto the domains $(u, \eta) \in [-1, +1] \times [-1, +1]$ through suitable coordinate transformations. Common transformations for this purpose include $u = \cos n_u \theta$ ($\eta = \cos n_\eta \phi$) where (n_u, n_η) are real numbers determined by the structure of the potential. These transformations are applicable to many forms of the potential with the popular values of n being either 1 or 2. For $n_\eta = 1$, for example, (1) assumes the form

$$\left[-\hat{T}_r - \frac{1}{r^2} \left(\hat{T}_\eta + \frac{1}{4} \right) + V(r, \eta) \right] \Phi(r, \eta) = E\, \Phi(r, \eta)\,, \tag{3}$$

whereas equation (2) takes the form

$$\left\{ -\hat{T}_r - \frac{1}{r^2} \left[4\, \hat{T}_u + \frac{2}{1-u} \left(4\, \hat{T}_\eta + \frac{1}{4} \right) + \frac{1}{4} \right] + V(r, u, \eta) \right\} \Phi(r, u, \eta) = E\, \Phi(r, u, \eta)\,, \tag{4}$$

when $n_u = 2$ and $n_\eta = 2$. In these equations the notation

$$\hat{T}_r = \frac{\partial^2}{\partial r^2}\,, \qquad \hat{T}_u = \left(1 - u^2 \right) \frac{\partial^2}{\partial u^2} - u\, \frac{\partial}{\partial u}\,, \tag{5}$$

is used, with $\hat{T}_\eta$ similar to $\hat{T}_u$. Note that $\hat{T}_u$ has the exact form of the operator related to the Chebyshev polynomials of the first kind, which also are a special case of the classical Jacobi polynomials [14]. The Lagrange basis functions used to evaluate the matrix elements of the Hamiltonian in (2) are discussed in the next section.

3. The Lagrange-mesh matrix elements

Bases expansions in the Lagrange-Laguerre and Lagrange-Jacobi functions, defined respectively on the Laguerre and Jacobi meshes, are used to approximate the solution to (2). Only the properties of the Lagrange-mesh method relevant to this work are indicated in this section. Details of these meshes as well as the principles of the Lagrange-mesh method are discussed by Baye [8].

The Jacobi mesh is defined by the zeros z_j ($j = 1, 2, 3, \ldots, N$) of the Jacobi polynomials $P_N^{\alpha,\beta}(z)$ of order N. The Lagrange-Jacobi functions defined on this mesh can be regularized by a factor $(1-z^2)^{\mu/2}$ [13], where μ is a free regularization parameter, to suppress singularities in the potentials that diverge at the boundaries. The resulting regularized Lagrange-Jacobi functions have the form

$$U_j(z) = (-1)^{N-j} \left[\frac{(1-z)^{\alpha+\mu}(1+z)^{\beta+\mu}}{(1-z_j^2)^{\mu-1}\,(2N+\alpha+\beta+1)\,h_N^{\alpha,\beta}} \right]^{1/2} \frac{P_N^{\alpha,\beta}(z)}{z-z_j} \tag{6}$$

where $h_N^{\alpha,\beta}$ is the normalizing constant of the Jacobi polynomials. The matrix elements for the angular operator (5), constructed with the regularized Lagrange-Jacobi functions $U_j(z)$, have the form [13]

$$\begin{aligned} T_{ij}^z &= \left\langle U_i(z) \left| \left[(1-z^2)\,\frac{\mathrm{d}^2}{\mathrm{d}z^2} - z\,\frac{\mathrm{d}}{\mathrm{d}z} \right] \right| U_j(z) \right\rangle \\ &= \begin{cases} (-1)^{i-j} \left(\dfrac{1-z_i^2}{1-z_j^2} \right)^{(\mu-1)/2} \left[\dfrac{(2\,\mu-1)\,z_i}{z_i-z_j} - \dfrac{2\,(1-z_i^2)}{(z_i-z_j)^2} \right] & ; \quad i \neq j \\ \dfrac{1-(2\,N+\alpha+\beta+1)^2}{12} + \dfrac{\omega_0+\omega_1\,z_i+\omega_2\,z_i^2}{6\,(1-z_i^2)} & ; \quad i = j \end{cases} \end{aligned} \tag{7}$$

where $\omega_0 = \alpha^2 + \beta^2 - 6\,\mu + 4$, $\omega_1 = \alpha^2 - \beta^2$ and $\omega_2 = 6\,(\mu-1)^2$. The parameters (α, β) define the Lagrange-Jacobi functions (6). These matrix elements are a special case of those of the Lagrange-Jacobi given in [13]. An appropriate choice of the (α, β) customizes the matrix elements to the Lagrange-Legendre, Lagrange-Chebyshev as well as the Lagrange-Gegenbauer functions.

There are two main types of Laguerre meshes determined by whether the Laguerre polynomials are functions of either r or r^2. For potentials of harmonic oscillator-type the r^2-dependence is convenient. The modified Laguerre mesh is defined by the zeros r_i^2 ($i = 1, 2, 3, \ldots, K$) of the Laguerre polynomials $L_K^\sigma(r^2)$ of order K. The Lagrange-Laguerre functions defined on this mesh are [8]

$$R_i(r) = (-1)^i \sqrt{\frac{2\,r_i^2}{h_K^\sigma}}\ \left(r^2\right)^{(2\,\sigma+1)/4}\ \mathrm{e}^{-r^2/2}\ \frac{L_K^\sigma(r^2)}{r^2-r_i^2} \tag{8}$$

where h_K^σ is the normalizing constant of the Laguerre polynomials. Note that this mesh depends on the parameter σ, which is usually chosen so that (8) displays the desired form at small values of r. The matrix elements for the radial kinetic energy operator constructed with the basis (8) are [8]

$$T_{ij}^r = \left\langle R_i(r) \left| -\frac{\mathrm{d}^2}{\mathrm{d}r^2} \right| R_j(r) \right\rangle = \begin{cases} (-1)^{i-j}\,\dfrac{8\,r_i\,r_j}{(r_i^2-r_j^2)^2} & ; \quad i \neq j \\ \dfrac{1}{3}\left[2\,(2\,K+\sigma+1) - r_i^2 - \dfrac{\sigma^2+5/4}{r_i^2} \right] & ; \quad i = j \end{cases} . \tag{9}$$

The parameter σ depends on the parameters (α, β) of the Lagrange-Jacobi functions discussed above. Note that the regularized modified Laguerre meshes [8] can also be used.

The solutions to (1) and (2) are developed through the basis expansion of the wave function. The following discussion focuses on (2) but can be readily reduced to that of (1) by simply omitting the dependency on u. To this end, the reduced wave function $\Phi(r, u, \eta)$ is expanded in the Lagrange functions bases of sizes (K, N, M),

$$\Phi(r, u, \eta) = \sum_{i=1}^{K} \sum_{j=1}^{N} \sum_{k=1}^{M} C_{ijk}\, R_i(r)\, U_j(u)\, U_k(\eta) \tag{10}$$

where C_{ijk} are the variational parameters, $R_i(r)$ the Lagrange-Laguerre functions (8), and $U_j(u)$ (and $U_k(\eta)$) the Lagrange-Jacobi functions (6). Pre-multiplying by Φ^*, applying the expansion (10) to equation (2), and integrating over the problem domain lead to the coupled algebraic equations

$$\sum_{i'=1}^{K} \sum_{j'=1}^{N} \sum_{k'=1}^{M} \Big[H^0_{ijk,i'j'k'} + V(r_i, u_j, \eta_k)\, \delta_{ii'}\, \delta_{jj'}\, \delta_{kk'} \Big]\, C_{i'j'k'} = E\, C_{ijk} \tag{11}$$

for the variational parameters. In these equations

$$H^0_{ijk,i'j'k'} = T^r_{ii'}\, \delta_{jj'}\, \delta_{kk'} - \frac{1}{r_i^2} \left[\left(4\, T^u_{jj'} + \frac{1}{4}\, \delta_{jj'} \right) \delta_{kk'} + \frac{2}{1-u_j} \left(4\, T^\eta_{kk'} + \frac{1}{4}\, \delta_{kk'} \right) \delta_{jj'} \right] \delta_{ii'} \tag{12}$$

are the kinetic energy matrix elements where the elements $T^u_{jj'}$ and $T^\eta_{kk'}$ are both given by (7) while $T^r_{ii'}$ are given by (9). Note that the elements $H^0_{ijk,i'j'k'}$ and $V(r_i, u_j, \eta_k)$ are the Gauss quadrature approximations of, respectively, the exact kinetic and potential energy matrix elements. Therefore, both matrices contribute integration errors to the numerical solutions [15]. Illustrative applications of and the accuracy attainable with the matrix elements (11) are discussed in the next section.

4. Applications

Illustrative applications of the presented Lagrange-mesh matrix elements are discussed for the quartic anharmonic oscillator in two dimensions and the double ring-shaped harmonic oscillator in three dimensions. Only the Gauss approximations of the matrix elements for the Hamiltonian are used in all the calculations presented. All the Lagrange meshes used are constructed with Gauss quadrature abscissas determined with accuracy of about 3×10^{-14} and the regularization parameter is set to $\mu = \frac{1}{2}$.

4.1. Quartic anharmonic oscillator

The two-dimensional quartic anharmonic oscillator potential in cylindrical polar coordinates has the form

$$V(r, \phi) = V_1\, r^2 + V_2\, r^4 \left[1 - 2\,(1-\nu)\, \sin^2\phi\, \cos^2\phi \right] ; \qquad r \in [0, \infty] , \quad \phi \in [0, 2\,\pi] , \tag{13}$$

where V_1, V_2 and ν are constants. Using the transformation $\eta = \cos 2\phi$ the potential is cast in the form

$$V(r, \eta) = V_1\, r^2 + V_2\, r^4 \left[1 - \tfrac{1}{2}\,(1-\nu)(1-\eta^2) \right] ; \qquad r \in [0, \infty] , \quad \eta \in [-1, +1] . \tag{14}$$

The system is solved using the Lagrange-Laguerre and Lagrange-Chebyshev functions where σ is determined by α_θ and β_θ. Note that the Chebyshev functions are the eigenfunctions of the

Table 1. Convergence of the energies for the first two states of the quartic anharmonic oscillator (13) with bases sizes (K, N). $V_1 = 1$ and $V_2 = 0.001$.

ν	(K, N)	E_{00}	E_{01}
-1	(3,6)	2.000 998 505 3	6.006 971 8
	(6,6)	2.000 998 505 469 824	6.006 970 242 132 808
	(7,3)[a]	2.000 998 505 469 810	6.006 970 242 132 821
0	(3,6)	2.001 497 385	6.010 463 0
	(6,6)	2.001 497 385 346 379	6.010 460 565 461 274
	(7,3)[a]	2.001 497 385 346 371	6.010 460 565 461 293
1	(3,6)	2.001 995 521 5	6.013 940 2
	(6,6)	2.001 995 522 094 719	6.013 936 098 189 642
	(7,3)[a]	2.001 995 522 094 708	6.013 936 098 189 653

[a] Results of [16] where N represents the size of the sub-problem.

kinetic energy operator of the system. To facilitate the comparison with the results of [16], the Schrödinger equation for this potential is solved with the parameters $V_1 = 1$, $V_2 = 0.001$ and $\nu = \{-1, 0, 1\}$, although the parameters (K, N) have a slightly different meaning [a]. Convergence tests with the bases sizes were conducted and the results are shown in table 1.

As can be seen in the table, the calculated energies converge rapidly with the increasing bases size. Results comparable with those of [16] are obtained with a basis of comparable size, $(K, N) = (6, 6)$. Note that in the treatment presented in [16] preconditioning specific to this potential is used before constructing the eigenvalue problem for the system. However, in the present work the system is readily transformed to a standard eigenvalue problem. In addition, the kinetic energy matrix elements presented in this work are applicable not only to the Chebyshev functions of the first kind. The application of the matrix elements with the Lagrange-Jacobi and the Lagrange-Gegenbauer functions is illustrated in the next subsection.

4.2. Double ring-shaped harmonic oscillator

The harmonic oscillator coupled with the Pöschl-Teller double ring-shaped potential is written in the form

$$\begin{aligned} V(r,\theta,\phi) &= r^2 + \frac{1}{r^2}\left[\frac{1}{\sin^2\theta}\left(\frac{a^2-\frac{1}{4}}{\sin^2\phi}+\frac{b^2-\frac{1}{4}}{\cos^2\phi}\right)+\frac{c^2-\frac{1}{4}}{\cos^2\theta}\right]; \\ & r\in(0,\infty], \qquad \theta\in[0,\tfrac{1}{2}\pi] \qquad \text{and} \qquad \phi\in[0,\tfrac{1}{2}\pi], \end{aligned} \tag{15}$$

where a, b and c are constants. The Schrödinger equation for this potential admits exact solutions [2] with eigenvalues

$$E_{ijk} = 2\,[\,2\,(\,i+j+k\,)+a+b+c+3\,] \tag{16}$$

for $i = 0, 1, 2, \ldots$, $j = 0, 1, 2, \ldots$, and $k = 0, 1, 2, \ldots$. Through the transformations $u = \cos 2\theta$ and $\eta = \cos 2\phi$ the potential is cast in the form

$$\begin{aligned} V(r,u,\eta) &= r^2 + \frac{2}{r^2}\left[\frac{2}{1-u}\left(\frac{1}{1-\eta}+\frac{1}{1+\eta}\right)+\frac{1}{1+u}\right]; \\ & r\in(0,\infty], \qquad u\in[-1,+1] \qquad \text{and} \qquad \eta\in[-1,+1] \end{aligned} \tag{17}$$

where, for this work, the potential parameters are set to $a = b = c = 3/2$. The system is solved using the Lagrange-Laguerre, Lagrange-Jacobi and Lagrange-Gegenbauer functions ($\alpha_\phi = \beta_\phi$). Note that α_θ is determined by α_ϕ and β_ϕ while σ is determined by α_θ and β_θ. Convergence tests with bases sizes were conducted and the results are shown in table 2 for $\alpha_\phi = \beta_\phi = 3/2$ and $\beta_\theta = 1$ and in table 3 for $\alpha_\phi = \beta_\phi = \beta_\theta = 3/2$. The errors

$$\epsilon_n = \left| \frac{E_n(\text{num}) - E_n(\text{anal})}{E_n(\text{anal})} \right| ,$$

of the numerical energies $E_n(\text{num})$ relative to the analytical energies $E_n(\text{anal})$, are also shown in the tables.

Table 2. Convergence of the energies for the first three states of the double ring-shaped harmonic oscillator with bases sizes $(K, N, M) = (15, 15, 15)$. $\alpha_\phi = \beta_\phi = 3/2$ and $\beta_\theta = 1$.

n	$E_n(\text{num})$	$E_n(\text{anal})$	ϵ_n
0	14.998	15.0	1.10(-04)
1	18.995	19.0	2.85(-04)
1	18.997	19.0	1.41(-04)
1	18.998	19.0	8.77(-05)
2	22.988	23.0	5.27(-04)
2	22.992	23.0	3.62(-04)
2	22.995	23.0	2.36(-04)
2	22.996	23.0	1.69(-04)
2	22.997	23.0	1.17(-04)
2	22.998	23.0	7.62(-05)

Practically no computational time is spend on constructing the matrices and it is immediately noticed, in the tables, that the degeneracies of the states are correctly reproduced. In general

Table 3. Same as in table 2, with bases sizes $(K, N, M) = (3, 3, 3)$ and $\alpha_\phi = \beta_\phi = \beta_\theta = 3/2$.

n	$E_n(\text{num})$	$E_n(\text{anal})$	ϵ_n
0	14.999 999 999 999 978	15.0	1.42(-15)
1	18.999 999 999 999 978	19.0	1.12(-15)
1	19.000 000 000 000 000	19.0	0.00(+0)
1	19.000 000 000 000 017	19.0	9.35(-16)
2	22.999 999 999 999 986	23.0	6.18(-16)
2	22.999 999 999 999 996	23.0	1.54(-16)
2	23.000 000 000 000 000	23.0	0.00(+0)
2	23.000 000 000 000 004	23.0	1.54(-16)
2	23.000 000 000 000 004	23.0	1.54(-16)
2	23.000 000 000 000 004	23.0	1.54(-16)

the numerical energies converge, though quite slowly, with the increasing basis size when the parameters of the Lagrange-Jacobi functions are chosen arbitrarily. For example, with the parameter set $\alpha_\phi = \beta_\phi = 3/2$ and $\beta_\theta = 1$, all the calculated energies, given in table 2, are reproduced to about $\epsilon_n \approx 10^{-4}$ with the bases sizes $(K, N, M) = (15, 15, 15)$. However, when the correct values of the parameters of the Lagrange functions ($\alpha_\phi = \beta_\phi = \beta_\theta = 3/2$) are used, the calculated energies, shown in table 3, are reproduced to machine accuracy with very low bases sizes $(K, N, M) = (3, 3, 3)$.

5. Conclusions

The Lagrange-mesh method was used to solve the Schrödinger equation in polar coordinates. The method readily transforms the Schrödinger equation to an eigenvalue problem and is applicable to any well behaved potential functions. The recently developed Lagrange-Jacobi matrix elements were specialized to the Lagrange-Chebyshev elements to represent the angular kinetic energy matrix elements. The method was then applied to the quartic anharmonic oscillator in two-dimensions as well as the double ring-shaped harmonic oscillator in three-dimensions. The results show that convergence to the correct solutions with increasing basis size is generally slow but reasonable when the basis parameters (α, β) are chosen consistent with the eigenfunctions of the kinetic energy operator. However, eigenvalues for the systems are reproduced to within machine accuracy when the parameters are chosen appropriately.

References

[1] Flügge S 1999 *Practical quantum mechanics* (Berlin: Springer-Verlag)
[2] Bachkhaznadji A, Lassaut M and Lombard R J 2009 *J. Phys. A: Math. Theor.* **42** 065301
[3] Colbert D T and Miller W H 1992 *J. Chem. Phys.* **96** 1982–1991
[4] Chen Z and Goldman S P 1992 *Phys. Rev. A* **45**(3) 1722–1731
[5] Ram-Mohan L 2002 *Finite Element and Boundary Element Applications in Quantum Mechanics* (New York: Oxford University Press)
[6] Amore P and Fernández F M 2010 *Phys. Scr* **81** 045011
[7] Al-Jaber S M 2010 *Nuovo Cimento* **125** 1099–1108
[8] Baye D 2015 *Phys. Rep.* **565** 1–107
[9] Descouvemont P, Daniel C and Baye D 2003 *Phys. Rev. C* **67**(4) 044309
[10] Lacroix G, Semay C and Buisseret F 2012 *Phys. Rev. E* **86**(2) 026705
[11] Baye D, Filippin L and Godefroid M 2014 *Phys. Rev. E* **89**(4) 043305
[12] Vincke M, Malegat L and Baye D 1993 *J. Phys. B: At. Mol. Opt. Phys.* **26** 811
[13] Rampho G J 2016 *J. Phys. A: Math. Theor.* **49** 27501
[14] Abramowitz M and Stegun I 1965 *Handbook of mathematical functions* (New York: Dover)
[15] Szalay V 1993 *J. Chem. Phys.* **99** 1978–1984
[16] Taşeli H, Erhan İ M and Uğur Ö 2002 *J. Math. Chem.* **32** 323–338