

Mesh-Free Radial Basis Functions Method for the Accurate Numerical Solution of the Radial Schrödinger Equation: I- Bound States

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Abstract. We present a meshless method based on the thin plate radial basis functions for an accurate and stable numerical solution of the radial Schrödinger equation for the bound-states.

Keywords: Radial Schrödinger equation, Bound states, eigenvalue, Meshless methods, Radial basis functions (RBF), thin-plate spline.

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INTRODUCTION

The analytical and numerical solution of the wave equations (relativistic or non-relativistic) have taken a great deal of interest and many different attempts have been used to obtain the energy eigenvalues from the wave equations exactly or numerically for non zero angular momentum quantum number ($l \neq 0$) for a given potential [1, 2, 3, 4, 5, 6, 7, 8, 9]. In this paper, we aim to solve the radial Schrödinger equation by using a mesh-free method called radial basis functions (RBF) method and show the results of this method for the Hulthén potential for any l -value. We also compare our results with those published in the literature in order to show the accuracy and effectiveness of the method. A programme has been written in Mathematica 6 [10] in order for the calculations and the programme can be obtained from authors upon request.

The motion of a particle with the mass μ in the spherically symmetric potential is described in the spherical coordinates and by defining $\Psi_{nlm}(r, \theta, \phi) = R_{nl}(r)Y_{lm}(\theta, \phi)$ with $R_{nl}(r) = \frac{u_{nl}(r)}{r}$, the following Schrödinger equation in natural units can be obtained:

$$\left[\frac{d^2}{dr^2} - 2\mu (V_{eff}(r) - E_{n,l}) \right] u_{n,l}(r) = 0 \quad (1)$$

where $l = 0, 1, 2, \dots$ denotes the orbital angular-momentum quantum number and $n = 0, 1, 2, \dots$ denotes the principal quantum number that shows the number of nodes of the bound-state wave function within $(0, \infty)$.

The normalization, initial and boundary conditions on the wave function are given as

$$\int_0^{\infty} dr [u_{n,l}(r)]^2 = 1, \quad \lim_{r \rightarrow 0} u(r) = r^{l+1}, \quad \text{and} \quad \lim_{r \rightarrow \infty} u(r) = 0. \quad (2)$$

In this paper, we demonstrate the application of the RBF method for the Hulthén potential as an example. The Hulthén potential [11] is given by

$$V_H(r) = -Ze^2\delta \frac{e^{-\delta r}}{1 - e^{-\delta r}} \quad (3)$$

where Z and δ are respectively the atomic number and the screening parameter, determining the range for the Hulthén potential. The Hulthén potential behaves like the Coulomb potential near the origin ($r \rightarrow 0$), but in the asymptotic region ($r \gg 1$), the Hulthén potential decreases exponentially, so its capacity for bound states is smaller than the Coulomb potential [4]. The effective potential in Eq. 1 is

$$V_{eff}(r) = V_H(r) + V_l(r) = -Ze^2\delta \frac{e^{-\delta r}}{1 - e^{-\delta r}} + \frac{l(l+1)\hbar^2}{2\mu r^2} \quad (4)$$

where $V_l(r) = \frac{l(l+1)\hbar^2}{2\mu r^2}$ is known as the centrifugal term and the reduced mass $\mu = \frac{m_1 m_2}{m_1 + m_2}$. This effective potential can not be solved analytically for $l \neq 0$ because of the centrifugal term. Therefore, we look for the numerical solution of the Schrödinger equation with this potential using RBF method in the next section.

SOLUTION WITH RBF METHOD

The approximation of a function $u_{n,l}(x)$, using RBF, may be written as a linear combination of N radial functions:

$$u_{n,l}(x) \simeq \sum_{j=1}^N \lambda_j \varphi(r_j) \quad (5)$$

where $r_j = \|x, x_j\|$ is the Euclidean norm. The collation method is used by applying the above equation at every point $i = 1, \dots, N$, giving:

$$u_{n,l}(x_i) \simeq \sum_{j=1}^N \lambda_j \varphi(r_{ij}) \quad i = 1, \dots, N \quad (6)$$

where $r_{i,j} = \sqrt{(x_i - x_j)^2}$, N is the number of data points, λ 's are coefficients to be determined and φ is the radial basis function. Some commonly used RBFs are given in Table 1 and the details of the method can be found in ref [12, 13].

TABLE 1. Commonly used radial basis functions

Polynomial (Rn)	$\phi(r) = r^n$, n odd
Thin Plate Spline (TPSn)	$\phi(r) = r^n \log r$, n even
Multiquadric (MQ)	$\phi(r, \epsilon) = \sqrt{1 + (\epsilon r)^2}$
Gaussian (GS)	$\phi(r, \epsilon) = e^{-(\epsilon r)^2}$

If we insert the approximation (6) into the closed form of Eq. 1, we get:

$$H \sum_{j=1}^N \lambda_j \varphi(r_{ij}) - E \sum_{j=1}^N \lambda_j \varphi(r_{ij}) = 0 \quad (7)$$

Eq. (7) in a matrix form we have

$$\begin{bmatrix} H\varphi_{11} - E\varphi_{11} & \cdots & \cdots & H\varphi_{1N} - E\varphi_{1N} \\ H\varphi_{21} - E\varphi_{21} & \cdots & \cdots & H\varphi_{2N} - E\varphi_{2N} \\ \vdots & \ddots & & \vdots \\ H\varphi_{N1} - E\varphi_{N1} & \cdots & \cdots & H\varphi_{NN} - E\varphi_{NN} \end{bmatrix} \begin{bmatrix} \lambda_1 \\ \lambda_2 \\ \vdots \\ \lambda_N \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix} \quad (8)$$

Applying the initial and boundary conditions given by equation (2), we get:

$$\begin{bmatrix} \varphi_{11} & \cdots & \cdots & \varphi_{1N} \\ H\varphi_{21} - E\varphi_{21} & \cdots & \cdots & H\varphi_{2N} - E\varphi_{2N} \\ \vdots & \ddots & & \vdots \\ \varphi_{N1} & \cdots & \cdots & \varphi_{NN} \end{bmatrix} \begin{bmatrix} \lambda_1 \\ \lambda_2 \\ \vdots \\ \lambda_N \end{bmatrix} = \begin{bmatrix} r_1^{l+1} \\ 0 \\ \vdots \\ 0 \end{bmatrix} \quad (9)$$

In order to determine the interpolation coefficients $(\lambda_1, \lambda_2, \dots, \lambda_N)$, the Gaussian elimination method with partial pivoting is generally used and the λ 's are back-substituted to get an approximation of $u(x)$. It is also possible to use Mathematica subprograms such as LinearSolve for these calculations. After finding the wave function, in order to find the energy eigenvalues, we look at the sign change of the wave function inside the potential well. The energy eigenvalue, E_{nl} , is the highest value that changes n times the sign of wave function at given l value.

The results obtained by using above-described RBF method is shown in Table 2 in comparison with the results from literature. As it can be perceived from the results, RBF method is very effective and accurate to obtain the bound state energy eigenvalues for both low and high screening parameters. Although we present only the results of the Hulthén potential in this short paper, the method can be applied to any arbitrary potential. Different type of potentials are included in the programme which can be obtained from the authors.

In sum, it is konwn that the numerical solution of radial Schrödinger equation has been a long standing and challenging problem and many numerical methods that attempt to find stable and accurate solutions have had to resort to artificial methods to stabilize the solution. In this work, we present that RBF method provides accurate results and it is very easy to implement. Extension of this method to the scattering problems would be interesting and the work is in progress.

Note: Mathematica 6 programme for the energy eigenvalues using RBF method can be obtained by sending an e-mail to boztosun@erciyes.edu.tr .

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TABLE 2. Energy eigenvalues of the Hulthén potential obtained by using RBF method as a function of the screening parameter for $2p$, $3p$ and $3d$ states in atomic units ($\hbar = \mu = e = 1$) and for $Z = 1$ in comparison with other methods.

	δ	RBF	AIM [4]	SUSY [5]	Numerical [6]	Variational [6]	Shifted [7]
2p	0.025	0.1127608	0.1128125	0.1127605	0.1127605	0.1127605	
	0.050	0.1010428	0.1012500	0.1010425	0.1010425	0.1010425	0.1010424
	0.075	0.0898509	0.0903125	0.0898478	0.0898478	0.0898478	
	0.100	0.0791797	0.0800000	0.0791794	0.0791794	0.0791794	0.0791794
	0.150	0.0594418	0.0612500	0.0594415	0.0594415	0.0594415	
	0.200	0.0419373	0.0450000	0.0418854	0.0418860	0.0418860	0.0418857
	0.250	0.0266117	0.0312500	0.0266060	0.0266111	0.0266108	
	0.300	0.0140045	0.0200000	0.0137596	0.0137900	0.0137878	
	0.350	0.0037931	0.0112500	0.0036146	0.0037931	0.0037734	
3p	0.025	0.0437069	0.0437590	0.0437068	0.0437069	0.0437069	
	0.050	0.0331646	0.0333681	0.0331632	0.0331645	0.0331645	0.03316518
	0.075	0.0239398	0.0243837	0.0239331	0.0239397	0.0239397	
	0.100	0.0160538	0.0168056	0.0160326	0.0160537	0.0160537	0.01606772
	0.150	0.0044660	0.0058681	0.0043599	0.0044663	0.0044660	
3d	0.025	0.0436030	0.0437587	0.0436030	0.0436030	0.0436030	
	0.050	0.0327532	0.0333681	0.0327532	0.0327532	0.0327532	0.0327532
	0.075	0.0230317	0.0243837	0.0230306	0.0230307	0.0230307	
	0.100	0.0144855	0.0168055	0.0144832	0.0144842	0.0144842	0.0144842
	0.150	0.0013960	0.0058681	0.0132820	0.0013966	0.0013894	

REFERENCES

1. O. Bayrak and I. Boztosun, *J. Phys. A: Math. Gen.* **39**, 6955 (2006).
2. M. Aygun, O. Bayrak and I. Boztosun, *J. Phys. B: At. Mol. Opt. Phys.* **40**, 537 (2007).
3. I. Boztosun, M. Karakoc, F. Yasuk and A. Durmus, *J. Math. Phys.* **47**, 062301 (2006).
4. O. Bayrak, G. Kocak and I. Boztosun, *J. Phys. A: Math. Gen.* **39**, 11521 (2006).
5. B. Gonul, O. Ozer, Y. Cancelik and M. Kocak, *Phys. Lett. A* **275**, 238 (2000).
6. Y. P. Varshni, *Phys. Rev. A* **41**, 4682 (1990).
7. A. Z. Tang and F. T. Chan, *Phys. Rev. A* **35**, 911 (1987).
8. M. Karakoc and I. Boztosun, *Int. J. Mod. Phys. E* **15**, 1253 (2006).
9. O. Bayrak, I. Boztosun and H. Ciftci, *Int. J. Quantum Chem.* **107**, 540 (2007).
10. Wolfram Research, Inc., Mathematica, Version 6, Champaign, IL (2007).
11. L. Hulthén, *Ark. Mat. Astron. Fys.* **28A** (1942) 5.
12. I. Boztosun and A. Charafi, *Engineering Analysis with Boundary Elements* **26**, 889 (2002).
13. A. Durmus, I. Boztosun, F. Yasuk, *Int. J. of Mod. Phys. C* **17**, 1151 (2006).