

ARBITRARY L -STATE SOLUTION OF SHIFTED DENG-FAN POTENTIAL BY INTERPOLATING WAVELET COLLOCATION METHOD

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The Solution of D-Dimensional Radial Schrödinger Equation with Shifted Deng-Fan (sDF) Potential has been Investigated by Interpolating Wavelet Collocation Method. The Wavelet Based Interpolating Collocation Scheme Can Extract the Bound State Spectrum of sDF Potential Efficiently without any Pekeris Type of Approximation of the Centrifugal term and it gives most Accurate Results in Bound State Eigen Solution. As an Application, Bound State Eigen-Energies of some Diatomic Molecules (H_2 , LiH, HCl, and CO) are Presented in Low and High-Lying States for any Arbitrary Values of $\{l, n\}$ and Compared with Existing best Results to show the Superiority of the Scheme.

Introduction

In this study, the bound state solution of d -dimensional radial Schrödinger equation with sDF molecular potential has been considered, which is given as^{1–5}.

$$V(r) = D_1 \left(1 - \frac{b}{e^{\alpha r} - 1} \right)^2 - D_2, \quad b = e^{\alpha r_e} - 1, \quad r \in \mathbb{R}^+. \quad (1)$$

where D_1 , D_2 represent the dissociation energy, α is the range of potential, r_e is equilibrium internuclear distance and r is internuclear distance. This potential is actually a modified form of originally Deng-Fan potential^{6–10}. Various scientific phenomena in science like diatomic molecular energy spectra, interactions between nuclei, the motion of the nucleons, and electromagnetic transitions in diatomic molecules can be explained through sDF potential model. The bound-state solutions of the relativistic and non-relativistic wave equations have been investigated by number of authors by different type of approximation of centrifugal term due to their significance application in

chemical physics, molecular spectroscopy, molecular physics, and related fields^{1–5}. The focus of this study is to investigate the numerical bound solution of the d -dimensional radial Schrödinger equation with sDF molecular potential without any Pekeris type approximation of centrifugal term for any arbitrary n, l by using interpolating wavelet collocation scheme with high accuracy. The collocation scheme based on interpolating wavelets^{11,12} generated by scale functions from the Daubechies family^{13,14} has been developed here to obtain highly accurate solutions of the NR-Schrödinger equation in a semi-infinite domain $\mathbb{R}^+$ containing sDF molecular potential. The energy eigenvalues for a set of homogeneous and heterogeneous diatomic molecules (H_2 , LiH, HCl and CO) for some arbitrary values of quantum numbers n and l obtained by the proposed scheme are provided here.

The work is organized as follows: In Section 2, a short overview of the interpolating wavelet basis and expansion of function in this basis are provided, along with an estimation of errors. The solution of the Schrödinger equation by using the interpolating wavelet collocation method with arbitrary angular momentum quantum numbers involving sDF molecular potential is

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obtained in Section 3. The results obtained by the scheme proposed here are demonstrated in Section 4. Finally, Section 5. gives a conclusion of the study presented here.

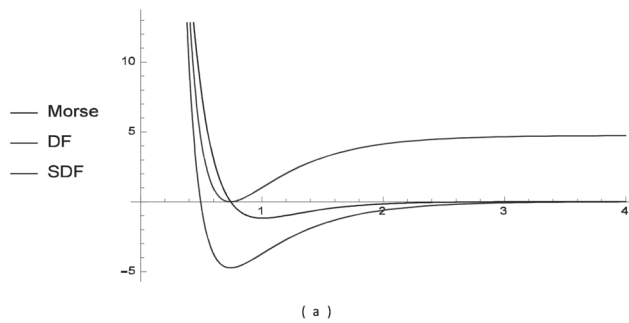


Fig. 1: Fig.(a) Variation of $V(r)$ with r of Morse, Deng-Fan(DF) and sDF potential for H_2 diatomic molecule.

Overview of Interpolating Wavelet

The fundamental theory of interpolating wavelets can be found in detail in literatures¹⁵⁻¹⁸. Here, some essential features of interpolating wavelet basis have been presented, as far as it is needed for our purpose.

1. The interpolating scale function $\Phi(x)$ and the wavelet $\Psi(x)$ ^{15,12} of compact support $(-2K+1, 2K-1)$, $K \in \mathbb{N}$ are defined at different scales as

$$\Phi_{j,k}(x) = \Phi(2^j x - k), \quad \Psi_{j,k}(x) = \Psi(2^j x - k) \quad (2)$$

2. Interpolating scale function, $\Phi(x)$ has vanishing moments for $i = 1, \dots, 2K-1$, i.e.

$$\int_{\mathbb{R}} x^i \Phi(x) dx = 0, \quad i = 0, \dots, 2K-1 \quad (3)$$

3. The interpolating wavelet function $\Psi(x)$ has vanishing moments for $i = 0, \dots, 2K-1$, i.e.

$$\int_{\mathbb{R}} x^i \Psi(x) dx = 0 \quad i = 0, \dots, 2K-1 \quad (4)$$

4. Any smooth functions $f \in L^2(\mathbb{R})$ can be approximated by

$$f(x) = f_i(x) = \sum_k f\left(\frac{k}{2^j}\right) \Phi_{j,k}(x) \quad (5)$$

The estimated error in the approximation in details given in Proposition 2.1 of¹⁷ as

$$E_j^{Est}[f]\left(\frac{k}{2^j}\right) \approx \left| \left(P_j f \right) \left(\frac{k}{2^j} \right) - \left(P_{j+1} f \right) \left(\frac{k}{2^j} \right) \right|;$$

$$E_j^{Est}[f] = \sup_{k \in A_j} E_j^{Est}[f]\left(\frac{k}{2^j}\right) \quad (2.5)$$

where $(P_j f)(x) = \frac{1}{2^j} \int_{\mathbb{R}} f(y) \Phi\left(\frac{y-x}{2^j}\right) dy$ and $\tilde{E}_j$ is an appropriate index set $(A_j = \{-2^{j+2}, \dots, 2^{j+2}\})$.

Formulation of Schrödinger Equation on The Interpolating Wavelet Basis

Let us consider the d-dimensional reduced radial Schrödinger equation

$$-\frac{\hbar^2}{2\mu} \frac{d^2 u}{dr^2}(r) + \frac{\hbar^2}{2\mu} \frac{(2l+d-1)(2l+d-3)}{4r^2} u(r) + V(r) u(r) = Eu(r), \quad r \in \mathbb{R}^+ \quad (3.1)$$

As there are some difficulties in the representation of unknown solution $u(r)$ directly in interpolating scale function basis $\{\Phi_{jk} | k \in \mathbb{Z}, j \in \mathbb{N}\}$, a special type of transformation has been used here, which is given by

$$r = \Theta(y) = e^{\frac{\pi}{2} \sinh y} \quad (3.2)$$

This transformation transforms the domain of the problem $\mathbb{R}^+$ into $\mathbb{R}$. The significance of this special transformation is that it acts as a contraction map that resolves the difficulties of partial support of the basis as well as counterbalance the singularities in the centrifugal term $1/r^2$. As a result, the scheme can effectively avoid Pekeris-type approximation.

Now, the approximation of the unknown solution $u(r)$ in Eq.(3.1) in the interpolating wavelet basis is given as

$$u_j^{Approx}(y) = \left(\phi_{jk}(y), k \in A_j^{(a,b)} \right) \cdot c_j \quad (3.3)$$

where $A_j^{(a,b)} = (2^j a, \dots, 2^j b)$ being an index set depending on the resolution j as well as limits a, b of the truncated domain in $\mathbb{R}$. Approximation $u_j^{Approx}(y)$ in (3.3) can now be used to transform this equation into a generalized matrix eigenvalue problem either by taking inner product of both sides with $(\phi_{jk}(y), k \in A_j^{(a,b)})$ (Galerkin approach) or by evaluating both sides at nodes $\left\{ \frac{k}{2^j}, k \in A_j^{(a,b)} \right\}$ (collocation method). The generalized matrix eigenvalue problem is obtained as

$$\mathcal{H}_j c_j = E^{Approx} \mathbb{Q}_j c_j \quad (3.4)$$

where the matrices H_j and Q_j are given by

$$\begin{aligned} \mathcal{H}_{jkl} = & -2^{2j} \Phi''(1-k) + \left\{ \frac{\pi}{2} \cosh\left(a + \frac{l}{2^j}\right) + \tanh\left(a + \frac{l}{2^j}\right) \right\} \\ & \times 2^j \Phi'(1-k) + \frac{\pi^2}{4} \cosh^2\left(a + \frac{l}{2^j}\right) \\ & \times \left\{ \frac{(l+2d-1)(l+2d-3)}{4} + \Theta\left(a + \frac{l}{2^j}\right)^2 \bar{V}\left(a + \frac{l}{2^j}\right) \right\} \\ & \times \Phi(l-k) \quad k, l = 0, \dots, 2^j(b-a). \end{aligned} \quad (3.5)$$

and

$$\begin{aligned} Q_{jl} = & \frac{\pi^2}{4} \Theta\left(a + \frac{l}{2^j}\right)^2 \cosh^2\left(a + \frac{l}{2^j}\right), \\ & l = 0, \dots, 2^j(b-a) \end{aligned} \quad (3.6)$$

respectively. Then the eigen spectrum of the matrices (H_j , Q_j) can be obtained directly by using any efficient library function in a computational software, e.g., “Eigensystem” in MATHEMATICA.

Results and Discussion

Here, the efficiency of the scheme has been established by the estimated errors for states $l = 0$ with a homogeneous diatomic molecule H_2 , where minimum

accuracy is 12 decimal places $\{n = 5, l = 0\}$ and maximum is upto 20 decimal places $\{n = 0, l = 0\}$. Then the energy spectrum of H_2 , LiH , CO , and HCl diatomic molecules have been computed for any arbitrary l and n that are presented in Table-1. The potential parameters for this calculation are taken from [2] directly and the conversion factors Hartree energy = 27.21138 eV, $\hbar c = 1973.269678 \text{ eV \AA}^0$ are given in NIST database 2018.

Conclusion

In this study, a highly accurate numerical solution of the Schrödinger equation has been obtained for the sDF potential by the use of an efficient interpolating wavelet collocation method without any Pekeris-type approximation of the centrifugal term. The method is found to be quite accurate for any high- and low-lying states as well as conventional choice of potential parameters. The estimated errors of H_2 diatomic molecules for $l = 0, 1, 2$ and numerical values of eigenenergies of (H_2 , LiH , HCl , and CO) diatomic molecules with sDF potential for different angular momentum l are demonstrated here. The scheme developed here may be easily extended to solve a variety of molecular models involving Morse, Manning-Rosen, and Hulthen type molecular potentials in a non-relativistic and relativistic manner, where other numerical schemes often face difficulties due to approximation of the centrifugal term. Work in this direction is in progress and will be reported shortly.

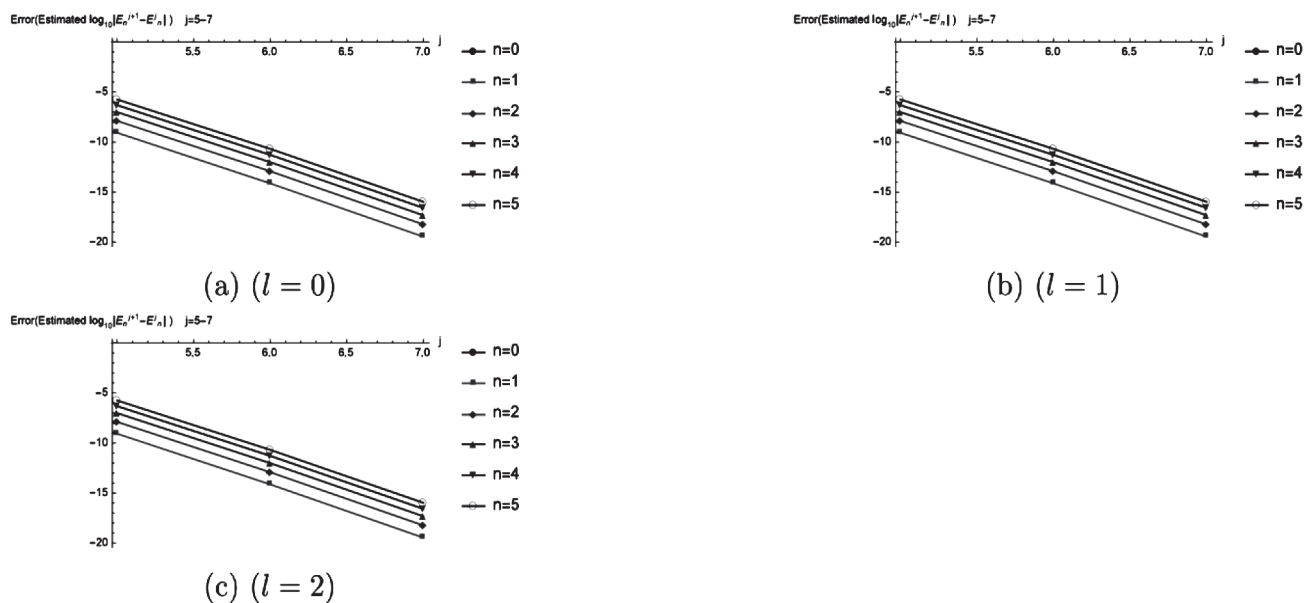


Fig. 2: Fig. (a-c) Plots of errors (Estimated errors in $\log_{10}$ scale) in the approximation of energies of H_2 diatomic molecules for different states ($n = 0, 1, \dots, 5$) with sDF potential for ($l = 0, 1, 2$) at different resolution ($j = 5 \text{ -- } 7$).

Table 1: Eigenenergies ($-E$) in eV of sDF potential for H_2 , LiH , HCl , and CO diatomic molecules.

States		H_2	LiH	HCl	CO
n	l	Present method	Present method	Present method	Present method
0	0	4.394623310799	2.411933956692	4.417049456662	11.080751382006
	3	4.308382401676	2.400977626288	4.401589021819	11.077894131112
	5	4.180761369696	2.384582844386	4.378427613816	11.073608605396
	7	4.000047672053	2.360985447627	4.345034184642	11.067419144394
3	0	2.640531716089	1.845674861914	4.417049456662	11.080751382006
	3	2.574791289592	1.836030355411	2.574791289592	1.836030355411
	5	2.477651600636	1.821601208812	3.274610251843	10.226192734042
	7	2.340410962034	1.800838642038	3.244867541264	10.220188803972
5	0	1.758473613071	1.516273362912	1.599511694466	9.688159630728
	3	1.704795431403	1.507467116153	3.295244368477	10.230349817504
	5	1.625616875073	1.494294207386	2.634120212385	9.681373564509
	7	1.514049905437	1.475343787733	2.606794334310	9.675493259971

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