



## Application of Formula Method for Bound State Problems in Schrödinger Equation

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**ABSTRACT:** By using Formula method for bound state problems, we have obtained the approximate analytical solution of the radial Schrödinger equation for Varshni potential model. The energy eigenvalues and the corresponding eigenfunctions are calculated in closed forms. In the process, eigen values for  $a = b = 1, a = -1, b = -2,$  and  $b = -1, a = -2$  for  $2p, 3p, 3d, 4p$  and  $4f$  states with three different values of the potential range were generated using the Varshni potential. Special cases of the potential are equally studied. Some numerical results have been presented which showed a good agreement with previous results obtained from another method.

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The study of exactly solvable problem has attracted much attention in theoretical physics since the development of quantum mechanics. For instance, the solutions of the non-relativistic Schrödinger equation for a hydrogen atom and a harmonic oscillator in three dimensions represent two typical examples in quantum mechanics (Schiff, 1955; Landau and Lifshitz, 1977). There are few traditional techniques or methods used to solve second-order differential equation in order to obtain the solutions of the quantum systems. These methods include Nikiforov-Uvarov method (Ebomwonyi *et al.*, 2017; Ikot *et al.*, 2015; Onate and Idiodi, 2015; Hamzavi and Ikhdair, 2012), asymptotic iteration method (Bayrak *et al.*, 2007; Falaye *et al.*, 2013; Bayrak and Boztosun, 2007; Ateser *et al.*, 2007), supersymmetry shape invariance and solvable potential (Zarrinkamar *et al.*, 2010; Jia *et al.*, 2011; Hassanabadi, 2011; Onate *et al.*, 2017), factorization method (Onyeaju *et al.*, 2016), new exact quantization rule (Dong and Gonzalez-Cisneros, 2008; Gu *et al.*, 2009) and others. Recently, Falaye *et al.* (2014) developed the Formula method for bound state problems from asymptotic iteration method. This method seems to be very effective, but the simplification in obtaining the energy equation is somehow technical; hence, resulting in little report on it in literature. This necessitates the present study; and in this paper, we intend to investigate the non-relativistic Schrödinger equation with the Varshni potential function in the framework of the Formula

method for bound state problems. To the best of our knowledge, this is the first time the Schrödinger equation is being studied with the Varshni potential function using the Formula method.

The Varshni potential function is given as (Varshni, 1957; Oluwadare and Oyewumi, 2017)

$$V(r) = a - \frac{abe^{-\delta r}}{r}, \quad (1)$$

Where,  $a$  and  $b$  are the potential strengths,  $\delta$  is the screening parameter which controls the shape of the potential energy curve and  $r$  is the internuclear separation. The Varshni potential function is a short range repulsive potential energy function that plays an important role in both chemical and molecular physics (Varshni, 1957). The potential was used by Kaxiras and Pandey to describe the 2-body energy portion of multi-body condensed matter. This potential is used generally to describe bound states of the interaction of systems and has been applied in both classical and modern physics. The Varshni potential function can be adjusted to adjustable Varshni potential function as shown in Eq. (2)

$$V(r) = a - \frac{\mathcal{V}be^{-\delta r}}{r}, \quad (2)$$

Where  $\mathcal{V}$  is an adjusted parameter. The adjustable Varshni potential function can be transformed into

other useful physical potential function. For instance, when the adjustable parameter  $\nu = 1$ , and

$$\lim_{a \rightarrow 0} V(r) = -\frac{be^{-\delta r}}{r}, \quad (3)$$

the adjustable Varshni function turns to Yukawa potential model. Similarly, when the adjustable parameter  $\nu = 0$ , the adjustable Varshni potential function becomes a constant potential

$$V(r) = a. \quad (4)$$

### MATERIALS AND METHODS

In this section, the bound state system was applied to calculate the energy equation and the wave function of the three dimensional radial Schrödinger equation with the Varshni potential function in Eq. (2) by employing the Formula method.

*Formula Method:* Given a second-order differential equation of the form

$$\left( \frac{d^2}{dr^2} + \frac{c_1 - c_2 s}{s(1 - c_3 s)} \frac{d}{ds} + \frac{\xi_1 s^2 + \xi_2 s + \xi_3}{s^2(1 - c_3 s)^2} \right) \psi(s) = 0, \quad (5)$$

Falaye et al. (2015), gave the condition for energy equation as

$$\alpha_1^2 = \left[ \frac{\alpha_0^2 - \alpha_1^2 - \left[ \frac{1-2n}{2} - \frac{1}{2c_3} \left( c_2 - \sqrt{(c_3 - c_2)^2 - 4\xi_1} \right) \right]^2}{2 \left[ \frac{1-2n}{2} - \frac{1}{2c_3} \left( c_2 - \sqrt{(c_3 - c_2)^2 - 4\xi_1} \right) \right]} \right]^2$$

(6)

Where

$$\alpha_0^2 = \frac{(1 - c_1) + \sqrt{(1 - c_1)^2 - 4\xi_3}}{2}, \quad (7)$$

$$\alpha_1^2 = \frac{1}{2} + \frac{c_1}{2} - \frac{c_2}{2c_3} + \sqrt{\left( \frac{1}{2} + \frac{c_1}{2} - \frac{c_2}{2c_3} \right)^2 - \frac{\xi_1}{c_3^2} - \frac{\xi_2}{c_2} - \xi_3}, \quad (8)$$

and the corresponding wave function is given as

$$\psi_n(s) = N_n s^{\alpha_0} (1-s)^{\alpha_1} {}_2F_1(-n, n+2\alpha_0+2\alpha_1; 2\alpha_0+1; c_3 s). \quad (9)$$

### RESULTS AND DISCUSSION

*Bound State Solutions:* In this section, we calculate the energy equation and the wave function of the three dimensional radial Schrödinger equation with the Varshni potential function. The time independent

Schrödinger equation incorporating the potential function  $V(r)$ , nonrelativistic energy  $E_{n\ell}$  is given as

$$\left[ \frac{d^2}{dr^2} + \frac{2\mu}{\hbar^2} \left( E_{n\ell} - V(r) - \frac{\ell(\ell+1)\hbar^2}{2\mu r^2} \right) \right] R_{n,\ell}(r) = 0, \quad (10)$$

where  $\ell$  is the angular momentum quantum number,  $n$  is the orbital quantum number,  $R_{n,\ell}(r)$  is the wave function,  $\mu$  is the reduced mass and  $\hbar$  is the reduced Planck constant. Due to the presence of the centrifugal term  $\frac{1}{r^2}$  in Eq. (10), we cannot obtain a

solution for  $\ell = 0$  state, therefore, we must apply an approximation scheme to deal with the centrifugal term. For short range potential, it is found that the following approximation

$$\frac{1}{r^2} \approx \frac{\delta^2}{(1 - e^{-\delta r})^2}, \quad (11)$$

is a good approximation to the centrifugal term which is valid for  $\delta \ll 1$ .

Now, substituting the potential in Eq. (1) and the approximation in Eq. (11) into Eq. (10) and by defining a variable of the form  $y = e^{-\delta r}$ , Eq. (10) becomes

$$\left[ \frac{d^2}{dy^2} + \frac{1-y}{y(1-y)} \frac{d}{dy} + \frac{Ay^2 + By + C}{[y(1-y)]^2} \right] R_{n,\ell}(y) = 0, \quad (12)$$

Where

$$A = \frac{2\mu E_{n,\ell}}{\delta^2 \hbar^2} - \frac{2\mu a}{\delta^2 \hbar^2} - \frac{2\mu ab}{\delta \hbar^2}, \quad (13)$$

$$B = -\frac{4\mu E_{n,\ell}}{\delta^2 \hbar^2} + \frac{4\mu a}{\delta^2 \hbar^2} + \frac{2\mu ab}{\delta \hbar^2}, \quad (14)$$

$$C = \frac{2\mu E_{n,\ell}}{\delta^2 \hbar^2} - \frac{2\mu a}{\delta^2 \hbar^2} - \ell(\ell+1). \quad (15)$$

Comparing Eq. (12) with Eq. (5), we deduced the following

$$\left. \begin{aligned} c_1 &= c_2 = c_3 = 1, \\ \alpha_0^2 &= \frac{2\mu a}{\delta^2 \hbar^2} - \frac{2\mu E_{n,\ell}}{\delta^2 \hbar^2} + \ell(\ell+1), \\ \alpha_1^2 &= (1 + \ell)^2. \end{aligned} \right\} \quad (16)$$

Substituting Eq. (16) into Eq. (6), we have energy equation of the Varshni potential function as

$$E_{n,\ell} = a + \frac{\delta^2 \ell (\ell + 1) \hbar^2}{2\mu} - \frac{\delta^2 \hbar^2}{2\mu} \left[ \frac{\frac{2\mu ab}{\delta \hbar^2} - \ell (\ell + 1) - (1 + n + \ell)^2}{2(1 + n + \ell)} \right]^2 \quad (17)$$

The corresponding wave function is given as

$$R_{n\ell}(y) = N_{n\ell} y^{\sqrt{\frac{2\mu a}{\delta^2 \hbar^2} - \frac{2\mu E_{n,\ell}}{\delta^2 \hbar^2} + \ell(\ell+1)}} (1-y)^{1+\ell} \times$$

$${}_2F_1 \left( -n, n + \frac{4\mu a}{\delta^2 \hbar^2} - \frac{4\mu E_{n,\ell}}{\delta^2 \hbar^2} + 2\ell^2 + 4\ell + 2; \frac{4\mu a}{\delta^2 \hbar^2} - \frac{4\mu E_{n,\ell}}{\delta^2 \hbar^2} + 2\ell^2 + 2\ell + 1; y \right). \quad (18)$$

In Table 1, we generated eigenvalues for Varshni potential with  $a = b = -1$ ,  $a = -1, b = -2$ , and  $b = -1, a = -2$  for 2p, 3p, 3d, 4p, 4d and 4f states with three different values of the potential range. It is observed that as the potential range increases, the energy of the system increases. Similarly, at constant value of  $a$ , the energy of the system decreases as  $b$ , the strength of the potential decreases. This same effect is observed when  $a$  and  $b$  is interchanged. The energy of the system is also found to be increasing as both the orbital and angular momentum quantum number increases respectively. In Table 2, we presented eigenvalues for adjusted Varshni potential and Yukawa potential for 1s, 2s, 2p, 3s, 3p and 3d states. The energy equation for these potentials were obtained in special cases. To test the accuracy of these

results, we compared the result of Yukawa potential with the result of Hamzavi et al. (2013) who used parametric NikiforovUvarov method. As it can be seen from the Table 2, our results are in good agreement with the previous result. However, our results indicated that the results for adjusted Varshni potential and Yukawa potential are equivalent as considered in the special cases.

*Special Cases:* Using the adjustable potential in Eq. (2), the energy equation above remains the same except that the adjustable parameter will appear. When the adjustable parameter  $\nu = 1$  and  $a = 0$ , the energy equation for the adjustable Varshni potential turns to the energy equation for the Yukawa potential as

$$E_{n,\ell} = \frac{\delta^2 \ell (\ell + 1) \hbar^2}{2\mu} - \frac{\delta^2 \hbar^2}{2\mu} \left[ \frac{\frac{2\mu b}{\delta \hbar^2} - \ell (\ell + 1) - (1 + n + \ell)^2}{2(1 + n + \ell)} \right]^2 \quad (19)$$

When the adjustable parameter  $\nu = 0$ , the energy equation for the adjusted Varshni potential becomes energy equation for constant potential as

$$E_{n,\ell} = a + \frac{\delta^2 \ell (\ell + 1) \hbar^2}{2\mu} - \frac{\delta^2 \hbar^2}{2\mu} \left[ -\frac{\ell (\ell + 1)}{2(1 + n + \ell)} - \frac{(1 + n + \ell)}{2} \right]^2 \quad (20)$$

**Table 1:** Bound state energy eigenvalues of the Varshni potential as a function of the screening parameter with  $2\mu = \hbar = 1$ .

State	$\delta$	$E_{n,\ell}$ $a = b = -1$	$E_{n,\ell}$ , $a = -1,$ $b = -2$	$E_{n,\ell}$ , $a = -2,$ $b = -1$
2p	0.001	-1.0617502	-1.2485002	-2.2485002
	0.050	-1.0256250	-1.1756250	-2.1756250
	0.100	-0.9900000	-1.1025000	-2.1025000
3p	0.001	-1.0271680	-1.1098902	-2.1098902
	0.050	-1.0006250	-1.0534028	-2.0534028
	0.100	-0.9802778	-1.0025000	-2.0025000
3d	0.001	-1.0269447	-1.1094470	-2.1094470
	0.050	-0.9867361	-1.0284028	-2.0284028
	0.100	-0.9469444	-0.9469444	-1.9469444
4p	0.001	-1.0150656	-1.0613781	-2.0613781
	0.050	-0.9951563	-1.0139062	-2.0139062
	0.100	-0.9900000	-0.9806250	-1.9806250
4d	0.001	-1.0149391	-1.0611266	-2.0611266
	0.050	-0.9851563	-0.9976563	-1.9976563
	0.100	-0.9625000	-0.9406250	-1.9406250
4f	0.001	-1.0147502	-1.0607502	-2.0607502
	0.050	-0.9725000	-0.9756250	-1.9756250
	0.100	-0.9306250	-0.8900000	-1.8900000

**Table 2:** Bound state energy eigenvalues of the adjusted Varshni and Yukawa potentials as a function of the screening parameter with  $2\mu = \hbar = 1$ .

State	$\delta$	$E_{n,\ell}, c = 3$ $a = -0.01,$ $b = 1$	$E_{n,\ell}, c = 1$ $a = 0,$ $b = -3$	Hamzavi et al. (2013)
1s	0.001	-2.258 500	-2.248 500	-2.248 500
	0.005	-2.252 500	-2.242 251	-2.242 251
	0.010	-2.245 025	-2.235 025	-2.235 025
2s	0.001	-0.571 001	-0.561 001	-0.561 001
	0.005	-0.565 625	-0.555 025	-0.555 025
	0.010	-0.557 600	-0.547 600	-0.547 600
2d	0.001	-0.570 250	-0.560 250	-0.560 250
	0.005	-0.561 256	-0.551 256	-0.551 256
	0.010	-0.550 025	-0.540 025	-0.540 025
3s	0.001	-0.258 502	-0.248 502	-0.248 502
	0.005	-0.252 556	-0.242 556	-0.242 556
	0.010	-0.245 225	-0.235 225	-0.235 225
3p	0.001	-0.258 168	-0.248 168	-0.248 168
	0.005	-0.250 867	-0.240 867	-0.240 867
	0.010	-0.241 803	-0.231 803	-0.231 803
3d	0.001	-0.257 500	-0.247 500	-0.247 500
	0.005	-0.247 506	-0.237 506	-0.237 506
	0.010	-0.235 025	-0.225 025	-0.225 025

**Conclusion:** In this study, the approximate solution of the Schrödinger equation is obtained using a suitable approximation to the centrifugal term in the framework of Formula method for bound state problem. By change of parameters, an adjusted Varshni potential model was transformed to Yukawa potential and constant potential respectively. The result obtained shows a good agreement with a previous result obtained by another method. This confirmed the accuracy of the unpopularly used Formula method for bound state problem.

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