On the Research Methodology of the Numerical Simulation of the Varshni Potential Model

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ABSTRACT

This study investigates the Varshni potential energy function V in a numerical analysis framework. A linear first order ordinary differential equation satisfying only deterministic parameterisation is constructed and its general and particular solutions are obtained. Impact analysis is carried out on the model using numerical simulations, to investigate the sensitivity of the model parameters under external random perturbations, and the influence of these changes on the potential function. Four random perturbation configurations are studied in 15 scenarios each, with 15 iterations of numerical simulations run for each case, using a range of initial conditions. For each iteration, the effect of the perturbation on the potential levels is computed. The numerical algorithms are implemented with MATLAB, and Python is used to analyse and plot the results. The results of this study indicate that the potential strength is increasingly sensitive to increasing random perturbations, thus causing unpredictable fluctuations in the system. Further, higher initial values of the screening parameter result in lower curvatures in the potential curves. This study concludes that variations in potential strength have direct differential effects on the periodicity and instability of interacting potential systems, while variations in the screening parameter have direct influence on the shape of the curves. It is recommended that the methods used in this research should be extended to studying the effects of varying the range and iteration steps of the initial conditions, and the influence of computation time delays on the outcome of the simulations.

Key words: *Varshni potential, numerical simulation, random perturbation, sensitivity, stability*

1. INTRODUCTION

Over the past seven decades, there have been tremendous studies on the empirical potential energy functions for molecular structures to obtain meaningful insights from molecular spectra and verify the presence and nature of various elements. Functions like Varshni potential (Cheng & Serb, 2009) and Deng-Fan potential (Deng & Fan, 1957) are usually applied and potential energy curves are drawn. A potential energy curve graphically represents the change in the potential energy of a molecule as a function of the distortion of the bond of the molecule from its equilibrium distance. These curves are necessary in the calculations of thermodynamic quantities, Franck-Condon factor, dissociation energy, and molecular parameters of diatomic molecules ground state (Ayaash, 2015).

In theoretical investigations on diatomic molecules, several approaches such as Rydberg-Klein-Rees (RKR) method and direct-potential-fit (DPF) procedure have been proposed and utilised in varying degrees of efficiency (Coxon & Hajigeorgiou, 1991; Bruhl et al., 1991; Hedderich et al., 1963; Surkus, 1997; Seto et al., 1999). A variety of analytical potential function forms have also been introduced and applied to particular molecular systems (Hajigeorgiou & Le Roy, 2000; Coxon & Hajigeorgiou, 1991; Bruhl et al., 1991; Hedderich et al., 1963; Surkus, 1997; Seto at al., 1999).

Potential functions have been explored widely in studies of the Klein-Gordon equation, the most suitably used wave equation for the treatment of spinless particles in relativistic quantum mechanics. With various methods such as the scattering state solutions of various exactly solvable potential models, the Klein-Gordon equation has been studied extensively to unlock insights into atomic structures, electronic configuration of atoms, resonance and diverse collisions processes. (Durmus &Yasuk, 2007; Saad, Hall & Ciftci, 2008; Dai, 2011; Ortakaya, 2012; Sun & Dong, 2012).

There are many other scientific applications that widely employ potential energy functions, such as the molecular modelling of novel properties at the nano-scale, and the simulation of mechanical properties like fluid flow, mass transport and heat transfer. The interaction energy between bonded atoms and non-bonded energy of interaction are described in terms of these potentials.

Of particular interest to us in this study is the famous Varshni potential function which is ubiquitous in diverse investigations of atomic and molecular physics. Varshni (1957) gave a comprehensive review of the classical potential energy functions of diatomic molecules. The Varshni potential is a short range repulsive potential energy function used in describing the bound states of interaction systems and has been applied in classical and modern physics (Oluwadare and Oyewumi, 2016).

In all the important investigations of potential functions, there have been no rigorous mathematical analyses of experimental data for the various potential models. Our motivation in this study is to implement numerical simulations to fully investigate the Varshni potential function, an exhaustive mathematical analysis of which has not been previously accomplished to the best of our knowledge. To this end, we shall analyse the differential effects of iteratively varying the screening parameter and the initial potential strength separately on the predicted potential levels.

2. MODEL AND FIRST INSIGHTS

2.1 Introduction

We shall begin by considering the modified form of the Varshni potential function, with equal scalar and vector Varshni potentials, given as (Varshni, 1959; Lim, 2009):

$$V_{VP}(r) = S_{VP}(r) = a\left[1 - \frac{b}{r}e^{-\alpha r}\right] \tag{2.1}$$

where r is the internuclear distance, a and b are the strengths of the potential, and α is the screening parameter which controls the shape of the potential energy curve.

Rewriting (2.1),

$$V(r) = a\left[1 - \frac{b}{r}e^{-\alpha r}\right] \tag{2.2}$$

Differentiating (2.2), we formulate a first-order ODE model such that $V(r_0) = V_0 > 0$

$$\frac{dV}{dr} = \left(\frac{ab}{r}e^{-\alpha r}\right)\left(\alpha + \frac{1}{r}\right) \tag{2.3}$$

From Equation (2.2),

$$\frac{ab}{r}e^{-\alpha r} = a - V \tag{2.4}$$

Therefore,

$$\frac{dV}{dr} = (a - V)\left(\alpha + \frac{1}{r}\right) \tag{2.5}$$

Equation (2.5) is an ordinary differential equation model of Varshni potential which we shall analyse in this study. We have narrowed down our investigations to the first order ODE formulation satisfying only deterministic parameterisation.

2.2 Simplifying Assumptions

The following key assumptions shall form the bedrock for the rest of this study:

i) The performance of the potential V depends on the performance of r.

ii) The internuclear equilibrium distance r between two interacting systems under the influence of the potential is always greater than zero.

iii) The value of the potential at every r_0 must be greater than zero, i.e., $V(r_0) = V_0 > 0$

2.3 Basic Theorems

In this Section we state two fundamental results from calculus, viz, continuity and differentiability, and demonstrate that our potential function indeed satisfies these properties.

Theorem 2.3.1 (Continuity) *We say that a function V is continuous at r_0 if and only if V is defined in an open interval I containing r_0 and*

$$\lim_{r \to r_0} V(r) = V(r_0)$$

If V is continuous at every $r \in I$, then it is continuous on I. Further, we say V is continuous on

iv) ***the open-closed interval*** $(a, b]$ *if and only if the left-hand limit*

$$\lim_{r \to b^-} V(r) = V(b) \text{ for every } a < r \leq b$$

v) ***the closed-open interval*** $[a, b)$ *if and only if the right-hand limit*

$$\lim_{r \to a^+} V(r) = V(a) \text{ for every } a \leq r < b$$

vi) ***the closed interval*** $[a, b]$ *if and only if Conditions (i) and (ii) both hold.*

Proof: We prove this theorem in the case of the Varshni potential function,

$$V(r) = a\left[1 - \frac{b}{r}e^{-\alpha r}\right]$$

From our assumptions in Section 2.2, the domain of V is the open-closed interval $(0, \infty]$. To show continuity on this interval, we first prove the general criterion of the foregoing theorem, that V is continuous on the open interval $(0, \infty)$:

$$\begin{aligned}\lim_{r \to r_0} V(r) &= \lim_{r \to r_0} a\left[1 - \frac{b}{r}e^{-\alpha r}\right] \\ &= a\left[1 - \frac{b}{r_0}e^{-\alpha r_0}\right] \\ &= V(r_0)\end{aligned}$$

Now, we prove the specific condition (i) that V is continuous on the open-closed interval $(0, \infty]$

$$\begin{aligned}\lim_{r \to \infty^-} V(r) &= \lim_{r \to \infty} a\left[1 - \frac{b}{r}e^{-\alpha r}\right] \\ &= a\left[1 - \frac{b}{\infty}e^{-\alpha \infty}\right] \\ &= V(\infty)\end{aligned}$$

In both cases, it can be easily shown that the converse is true. ■

Theorem 2.3.2 (Differentiability) *Suppose r_0 is an interior point in an interval I, and the function V is defined in I. Then V is differentiable at r_0 if the difference quotient*

$$\frac{V(r) - V(r_0)}{r - r_0}, \qquad r \neq r_0$$

approaches a limit $V'(r_0)$ as $r \to r_0$. The limit is called the derivative of V at r_0 and is defined by:

$$V'(r_0) = \lim_{r \to r_0} \frac{V(r) - V(r_0)}{r - r_0} \tag{2.6}$$

If V is differentiable at every $r \in I$, then we simply say V is a differentiable function.

***Proof*:** For convenience, we let $r = r_0 + h$, so that Definition (3.1) can be rewritten as

$$V'(r_0) = \lim_{h\to 0} \frac{V(r_0 + h) - V(r_0)}{h} \tag{2.7}$$

Then,

$$V(r_0) = a\left[1 - \frac{b}{r_0} e^{-\alpha r_0}\right]$$

$$V(r_0 + h) = a\left[1 - \frac{b}{r_0 + h} e^{-\alpha(r_0+h)}\right]$$

$$V(r_0 + h) = a\left[1 - \frac{b}{r_0 + h} e^{-\alpha r_0} e^{-\alpha h}\right]$$

$$V(r_0 + h) - V(r_0) = ab\left[\frac{e^{-\alpha r_0}}{r_0} - \frac{e^{-\alpha r_0} e^{-\alpha h}}{r_0 + h}\right]$$

So that

$$\begin{aligned}
V'(r_0) &= abe^{-\alpha r_0} \lim_{h\to 0} \frac{1}{h}\left[\frac{1}{r_0} - \frac{e^{-\alpha h}}{r_0 + h}\right] \\
&= abe^{-\alpha r_0} \lim_{h\to 0} \frac{1}{h}\left[\frac{1}{r_0} - \frac{e^{-\alpha h}}{r_0 + h}\right] \\
&= abe^{-\alpha r_0} \lim_{h\to 0} \frac{1}{h}\left[\frac{r_0 + h - r_0 e^{-\alpha h}}{r_0(r_0 + h)}\right] \\
&= abe^{-\alpha r_0} \lim_{h\to 0} \left[\frac{r_0 + h - r_0 e^{-\alpha h}}{h r_0(r_0 + h)}\right] \\
&= abe^{-\alpha r_0} \lim_{h\to 0} \left[\frac{r_0 - r_0 e^{-\alpha h}}{h r_0(r_0 + h)} + \frac{h}{h r_0(r_0 + h)}\right] \\
&= abe^{-\alpha r_0} \lim_{h\to 0} \left[\frac{1 - e^{-\alpha h}}{h(r_0 + h)} + \frac{1}{r_0(r_0 + h)}\right] \\
&= abe^{-\alpha r_0} \lim_{h\to 0} \left[\frac{1}{r_0 + h}\left(\frac{1 - e^{-\alpha h}}{h}\right) + \frac{1}{r_0(r_0 + h)}\right] \\
&= abe^{-\alpha r_0} \lim_{h\to 0} \left[\frac{1}{r_0 + h}\left(\frac{-\alpha(1 - e^{-\alpha h})}{-\alpha h}\right) + \frac{1}{r_0(r_0 + h)}\right] \\
&= abe^{-\alpha r_0} \lim_{h\to 0} \left[\frac{\alpha}{r_0 + h}\left(\frac{e^{-\alpha h} - 1}{-\alpha h}\right) + \frac{1}{r_0(r_0 + h)}\right]
\end{aligned}$$

It can be checked that a limit of the form $\lim_{x\to 0}\left(\frac{e^{kx} - 1}{kx}\right)$ both exists and is equal to unity. Thus,

$$V'(r_0) = abe^{-\alpha r_0} \lim_{h\to 0} \left[\frac{\alpha}{r_0 + h} + \frac{1}{r_0(r_0 + h)}\right]$$

$$= abe^{-\alpha r_0}\left[\frac{\alpha}{r_0}+\frac{1}{r_0^2}\right] \qquad \blacksquare$$

Definition 2.3.3 *A function V defined on the interval I is continuously differentiable on I (written as $V \in C^1(I)$) if it is differentiable on I and the derivative is continuous.*

Remark. Following the same procedure that we used in the proof of Theorem 2.3.1, we find that the derivative $V'(r)$ is also continuous on $(0, \infty]$. Thus, $V(r) \in C^1(0, \infty]$.

3. METHODS

In Section 2, we developed a linear ODE model for the Varshni potential function and studied some properties of the function. In this section, we shall formulate an initial value problem for our model, obtain general and particular solutions, and analyse the steady state solutions. Afterwards, we shall implement a numerical integration algorithm to investigate the differential effects of varying model parameters on the potential. We shall test for the sensitivity of the model parameters due to variations of the parameter values one at a time, and account for the behaviour of the 1st degree sensitivity such that dV/dr is always greater than zero.

3.1 Initial Value Problem

The initial value problem for our Varshni potential model is the pair

$$\frac{dV}{dr} = (a - V)\left(\alpha + \frac{1}{r}\right), \qquad r = r_0, \qquad V(r_0) = V_0 \tag{3.1}$$

Setting $K = \alpha + \frac{1}{r}$ in the first term and rearranging, we obtain the linear first order ODE

$$\frac{dV}{dr} + VK = aK \tag{3.2}$$

To solve this linear differential equation, we multiply through by its integrating factor e^{Kr} which reduces it to an exact differential equation as follows:

$$e^{Kr}\frac{dV}{dr} + VKe^{Kr} = aKe^{Kr}$$

$$\frac{d}{dr}(Ve^{Kr}) = aKe^{Kr} \tag{3.3}$$

Integrating,

$$Ve^{Kr} = \int aKe^{Kr}\,dr = ae^{Kr} + C$$

$$V(r) = a + Ce^{-Kr} \tag{3.4}$$

Equation (3.4) is the general solution of our differential equation model for the Varshni potential.

3.2 Steady State Solutions

From the general solution above, we observe that as $r \to \infty$, $V(r) \to a$. Therefore, the equilibrium value or steady-state solution, V_e, such that $dV/dr = 0$, is $V_e = a$. Let $D_1 = a$ and $D_2 = a + (V_0 - a)e^{K(r_0 - r)}$. Setting $D = D_1 - D_2$, we obtain another equilibrium solution

$$D = (a - V_0)e^{K(r_0 - r)} \tag{3.5}$$

Testing for the stability of the equilibrium solution D, we obtain the following three scenarios:

i) ***When*** $\boldsymbol{r = r_0}$: D reduces to $(a - V_0)$, and the steady state solution neither grows nor decays.

ii) ***When*** $\boldsymbol{r < r_0}$**:** $e^{K(r_0 - r)} \to \infty$ and D grows exponentially so that the solution becomes unstable

iii) ***When*** $\boldsymbol{r > r_0}$**:** $K(r_0 - r) \to -\infty$ and $D \to 0$, thus, D is asymptotically stable.

3.3 Particular Solution

Geometrically, the general solution of an ODE is a family of infinitely many solution curves, one for each value of the arbitrary constant C (Kreyszig, 2011). To find the particular solution, we use the initial conditions specified in our IVP viz, $r = r_0$, $V(r_0) = V_0$. Thus,

$$V_0 = V(r_0) = a + Ce^{-Kr_0} \tag{3.6}$$

Rearranging,

$$Ce^{-Kr_0} = V_0 - a$$

$$C = e^{Kr_0}(V_0 - a) \tag{3.7}$$

Therefore, the particular solution for this initial value problem is

$$\begin{aligned} V(r) &= a + e^{Kr_0}(V_0 - a)e^{-Kr} \\ \Longrightarrow V(r) &= a + (V_0 - a)e^{K(r_0 - r)} \end{aligned} \tag{3.8}$$

3.4 Sensitivity Analysis

Having obtained the general and particular solutions, and analysed the conditions for stability of the steady state solutions, we shall investigate the differential effects of varying the model parameters on the potential using a numerical integration algorithm, and test for the sensitivity of the model parameters due to variations of the parameter values one at a time.

We begin by simulating the model using a MATLAB ode45 algorithm. We study the fluctuations in the potential V under various perturbation conditions, by adding some randomness to a and α with an assumption that both parameters are subjectable to random perturbations. To accomplish

this, we declare five functions in the numerical integration algorithm, each containing the ODE model. The first defines the parameter values $r = 2.4,\ a = 0.15,\ \alpha = 0.15$. The second and third contain the values of a and α modified respectively by a low-perturbing random number generator:

$$\begin{cases} a = 0.15 + 0.01 \times \text{rand}(1) \\ \alpha = 0.15 \end{cases} \tag{3.9}$$

$$\begin{cases} a = 0.15 \\ \alpha = 0.15 + 0.01 \times \text{rand}(1) \end{cases} \tag{3.10}$$

The fourth and fifth functions contain values of a and α modified respectively by a relatively high-perturbing random number generator:

$$\begin{cases} a = 0.15 + 0.4 \times \text{rand}(1) \\ \alpha = 0.15 \end{cases} \tag{3.11}$$

$$\begin{cases} a = 0.15 \\ \alpha = 0.15 + 0.4 \times \text{rand}(1) \end{cases} \tag{3.12}$$

We implement the algorithm in each case of low and high perturbations of a and α, running 15 iterations for each simulation. For initial conditions, we use 15 values of internuclear distance r starting from 0 in steps of 1, and we choose a relative tolerance of 0.001. Annotated codes are included in Appendix 1.

We then compute the effect of such perturbations on the potential level using the formula

$$Effect = \left(\frac{V_{mod} - V}{V}\right) \times 100\% \tag{3.13}$$

where V_{mod} represents the modified value of the potential for each iteration.

In the case of a decrease in the potential, a depletion formula is implemented instead

$$Effect = \left(1 - \frac{V_{mod}}{V}\right) \times 100\% \tag{3.14}$$

4. APPLICATIONS

In this section, we present the results from Subsection 3.4 in which we quantified the effects of low and high perturbations of a and α on V.

5. NUMERICAL RESULTS

In this section, we present the results from Subsection 3.4 in which we quantified the effects of low and high perturbations of a and α on V.

Table 5.1: Quantifying the effect of a 0.01 random perturbation of a on V

Iterations	r	$V(r)$	$V_{mod}(r)$	$Effect$ (%)
1	0.0000	2.5000	2.5000	0.0000
2	1.0000	1.4828	1.4870	0.2823
3	2.0000	0.9067	0.9115	0.5297
4	3.0000	0.5794	0.5872	1.3340
5	4.0000	0.3936	0.4014	1.9791
6	5.0000	0.2883	0.2965	2.8563
7	6.0000	0.2285	0.2333	2.1148
8	7.0000	0.1945	0.1987	2.1382
9	8.0000	0.1753	0.1809	3.2271
10	9.0000	0.1643	0.1694	3.0587
11	10.0000	0.1581	0.1628	2.9600
12	11.0000	0.1546	0.1581	2.2691
13	12.0000	0.1526	0.1572	3.0098
14	13.0000	0.1515	0.1569	3.5865
15	14.0000	0.1508	0.1575	4.4276

Table 5.2: Quantifying the effect of a 0.4 random perturbation of a on V

Iterations	r	$V(r)$	$V_{mod}(r)$	$Effect$ (%)
1	0.0000	2.5000	2.5000	0.0000
2	1.0000	1.4828	1.5655	5.5718
3	2.0000	0.9067	1.0467	15.4448
4	3.0000	0.5794	0.7423	28.1120
5	4.0000	0.3936	0.5713	45.1410
6	5.0000	0.2883	0.4812	66.9264
7	6.0000	0.2285	0.4384	91.8694
8	7.0000	0.1945	0.3762	93.4053
9	8.0000	0.1753	0.3514	100.4816
10	9.0000	0.1643	0.3546	115.7934
11	10.0000	0.1581	0.3433	117.1047
12	11.0000	0.1546	0.3567	130.6675
13	12.0000	0.1526	0.3447	125.8338
14	13.0000	0.1515	0.3535	133.3743
15	14.0000	0.1508	0.3400	125.3742

Table 5.3: Quantifying the effect of a 0.01 random perturbation of α on V

Iterations	r	$V(r)$	$V_{mod}(r)$	$Effect$ (%)
1	0.0000	2.5000	2.5000	0.0000
2	1.0000	1.4828	1.4738	0.6095
3	2.0000	0.9067	0.8973	1.0332
4	3.0000	0.5794	0.5744	0.8723
5	4.0000	0.3936	0.3905	0.7971
6	5.0000	0.2883	0.2855	0.9546
7	6.0000	0.2285	0.2265	0.8681
8	7.0000	0.1945	0.1931	0.7485
9	8.0000	0.1753	0.1743	0.5580
10	9.0000	0.1643	0.1637	0.4013
11	10.0000	0.1581	0.1577	0.2731
12	11.0000	0.1546	0.1544	0.1651
13	12.0000	0.1526	0.1525	0.1021
14	13.0000	0.1515	0.1514	0.0674
15	14.0000	0.1508	0.1508	0.0416

Table 5.4: Quantifying the effect of a 0.4 random perturbation of α on V

Iterations	r	$V(r)$	$V_{mod}(r)$	$Effect$ (%)
1	0.0000	2.5000	2.5000	0.0000
2	1.0000	1.4828	1.1873	19.9323
3	2.0000	0.9067	0.6114	32.5696
4	3.0000	0.5794	0.3565	38.4800
5	4.0000	0.3936	0.2444	37.9063
6	5.0000	0.2883	0.1975	31.5011
7	6.0000	0.2285	0.1718	24.7958
8	7.0000	0.1945	0.1606	17.4264
9	8.0000	0.1753	0.1561	10.9436
10	9.0000	0.1643	0.1527	7.0860
11	10.0000	0.1581	0.1513	4.3266
12	11.0000	0.1546	0.1509	2.4142
13	12.0000	0.1526	0.1503	1.5484
14	13.0000	0.1515	0.1501	0.9038
15	14.0	0.1508	0.1501	0.5226

6. DISCUSSION

In Section 2.2, we made a fundamental assumption that the internuclear distance r between two interacting systems under the influence of the potential is always greater than zero. We tested this in our numerical simulation, beginning the iterations from $r = 0$. We found that indeed at this value, the perturbation effects of the model parameters on the potential were negligible. Also, dV had a value of $-\infty$ at $r = 0$.

The following are Python created plots for some specific scenarios that illustrate the 4 perturbation configurations we investigated, starting with the first configuration in which the potential strength a is varied on V by a 0.01 random perturbation, while keeping α at 0.15.

Figure 6.1 shows the potential energy curves for the two interacting potentials. The blue curve represents the initial behaviour when a and α both have values of 0.15. The red curve represents the response when a is varied by a 0.01 random perturbation while keeping α constant. It can be observed that there is negligible deviation from the initial behaviour under this configuration.

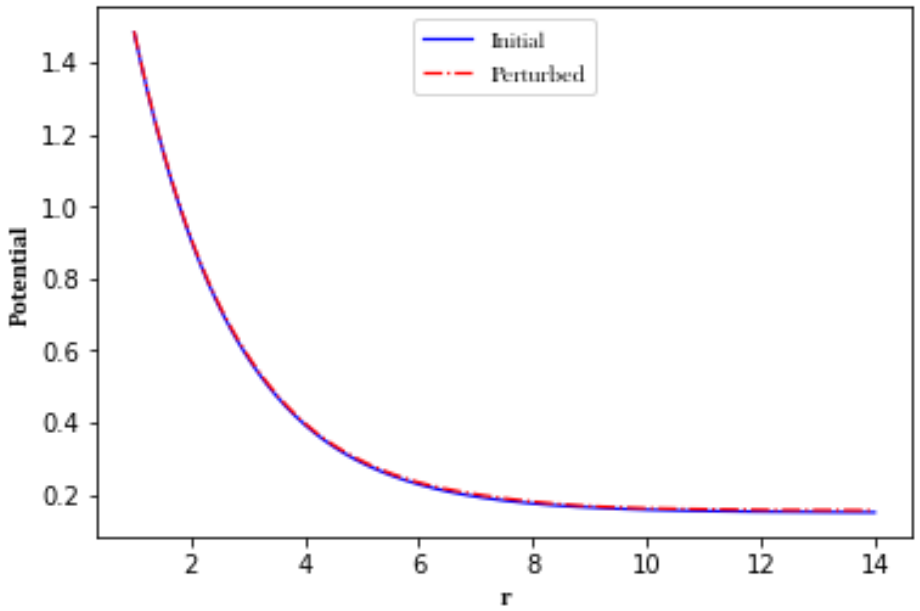


Figure 6.1: Variation of the potential level as a function of r under a 0.01 perturbation configuration of a

In Figure 6.2, dV is plotted against the two interacting potentials with the second under the same perturbation configuration as above. We observe that the red curve shows little deviation from the blue, just as in Figure 6.1, indicating that when a undergoes such a low random perturbation, the effect on V is small. However, the behaviour of the system changes dramatically when the initial value of the potential strength a is increased to 0.5. For the same data with which the above plots were generated, we observe stochastic trends for the low perturbation configuration.

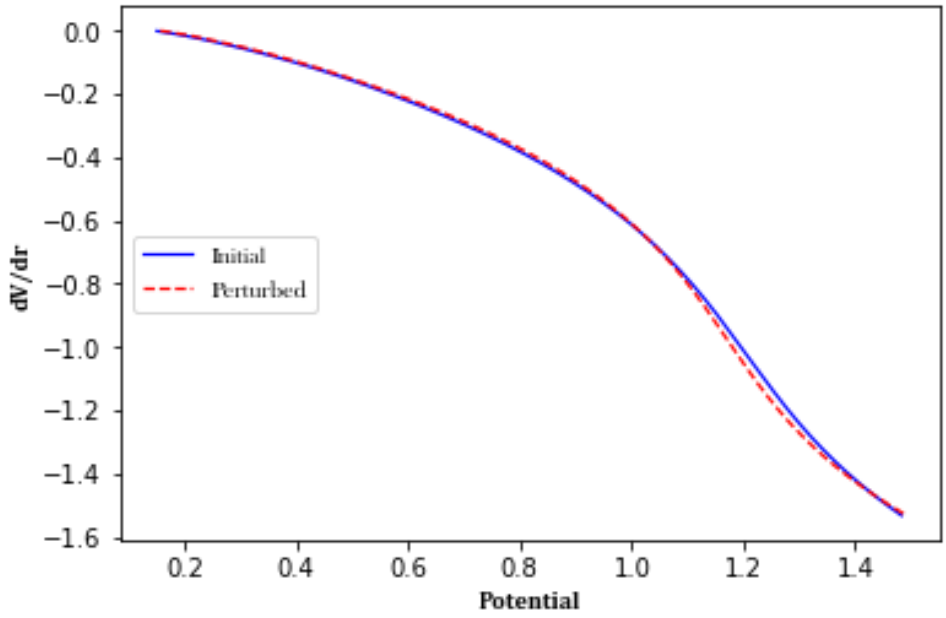


Figure 6.2: Differential effect of a 0.01 random perturbation configuration of a on the initial potential level

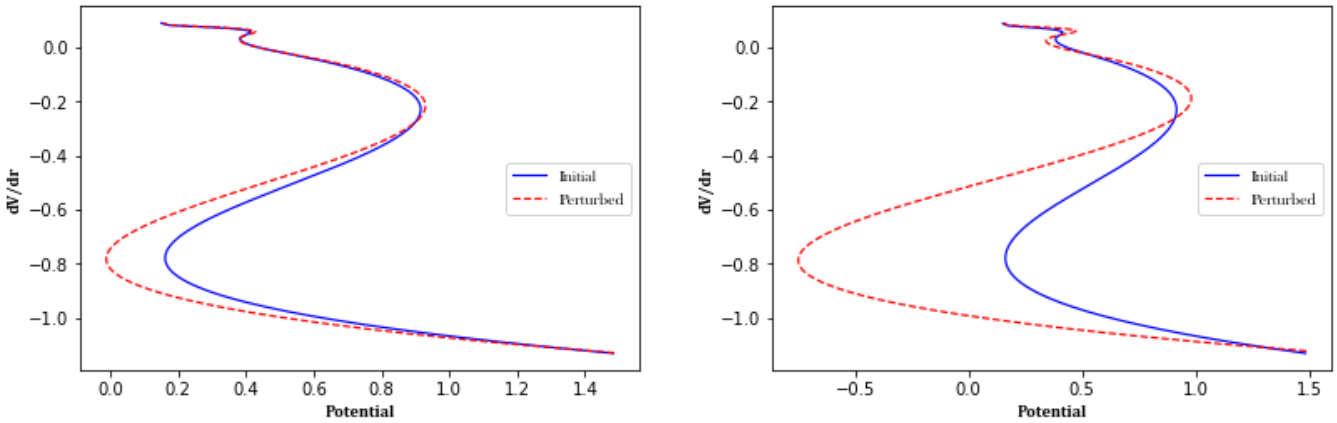


Fig 6.3 (a) and (b): Stochastic trends when a was increased to 0.5 and subjected to a 0.01 random perturbation configuration

We observe that the blue curve shows a more periodic behaviour at $a = 0.5$ than it does at $a = 0.15$, as the above plots indicate more crests and troughs and longer amplitudes. Further, when a is subjected to the 0.01 random perturbation configuration, the system behaves very stochastically. Comparing with Figure 6.2, this indicates that the potential strength a becomes increasingly sensitive to random fluctuations as its value increases.

Stronger trends are observed for a relatively higher perturbation configuration. In fact, when a is subjected to a 0.4 random perturbation, the deviation in the potential level increases drastically.

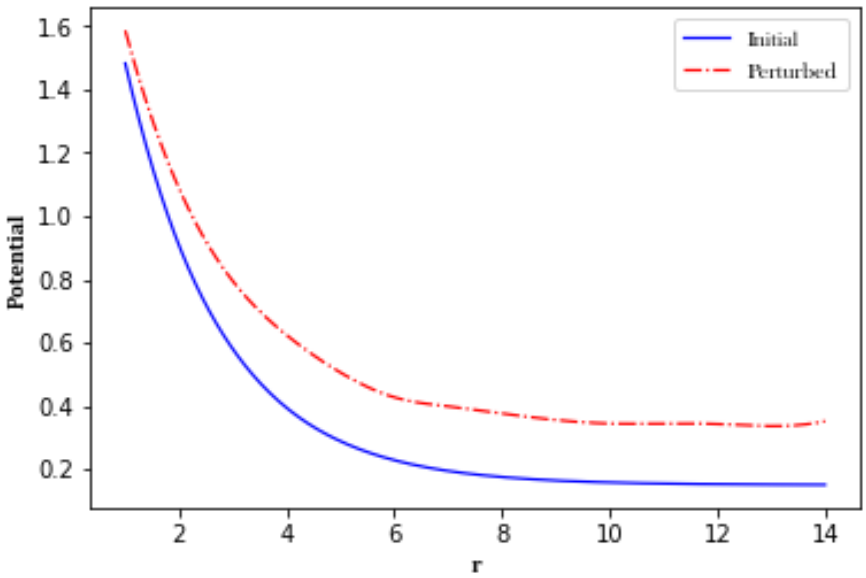
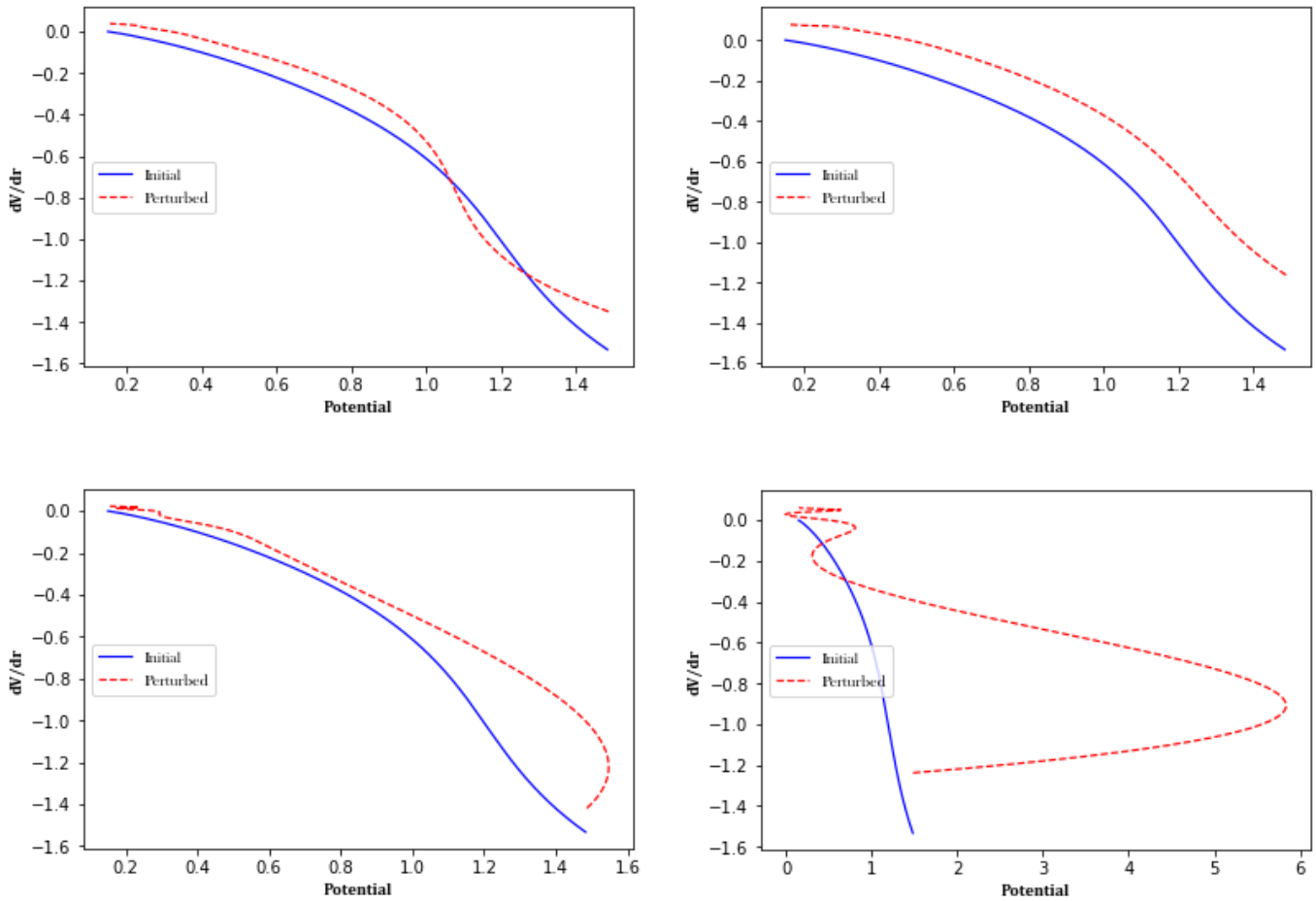


Figure 6.4: Variation of the potential levels as a function of r under a 0.4 perturbation configuration of a



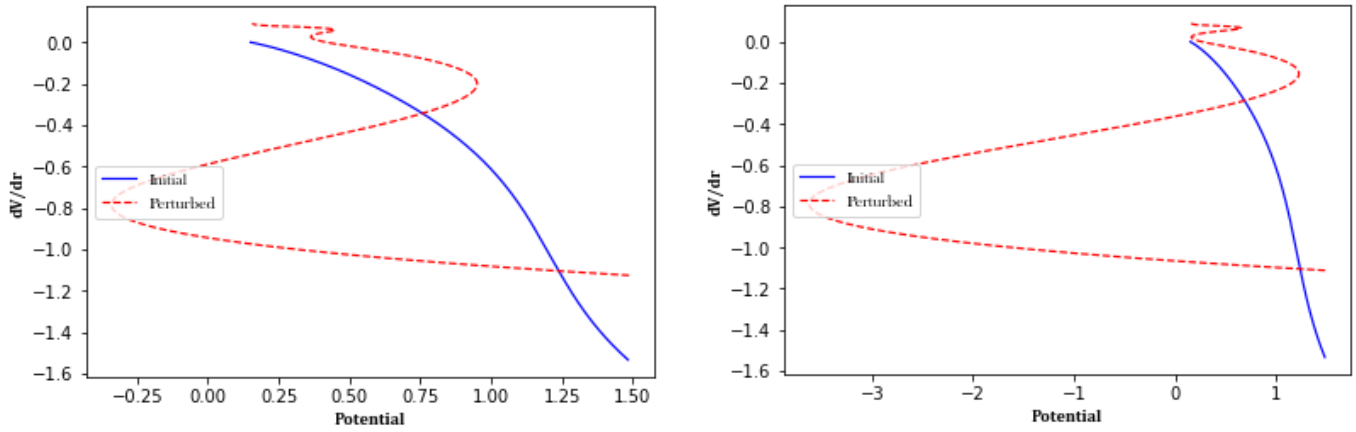


Fig 6.5 (a) - (f): Unstable stochastic trends when a was set to 0.15 and subjected to a 0.4 random perturbation configuration

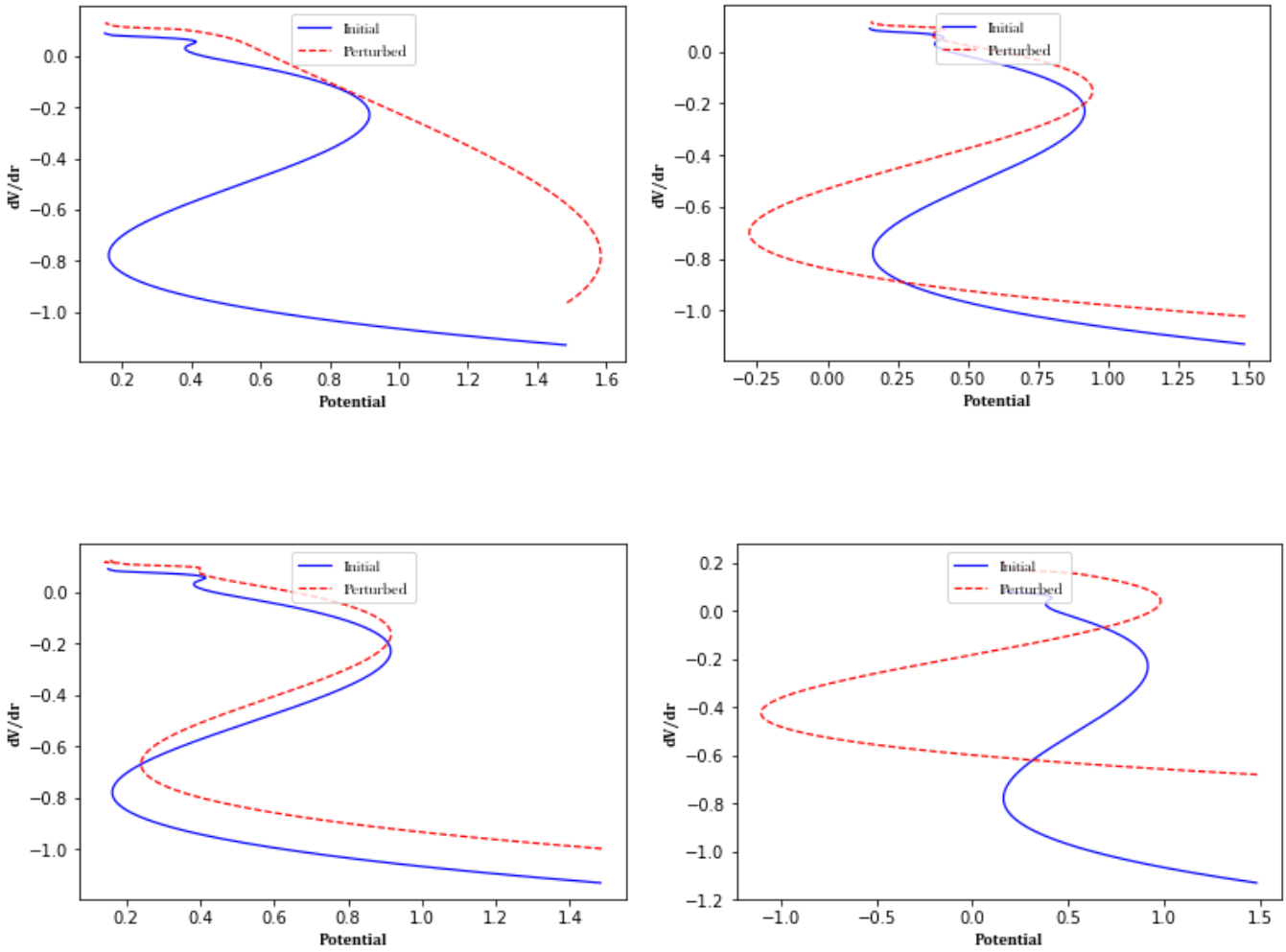


Fig 6.6 (a) - (d): Unstable stochastic trends when a was increased to 0.5 and subjected to a 0.4 random perturbation configuration

For low perturbation configurations of alpha, the trend is quite similar to Figure 6.1 and 6.2, as there is little to no deviation in the potential levels. However, for a relatively higher perturbation, stochastic trends are observed, similar in strength to the previous cases.

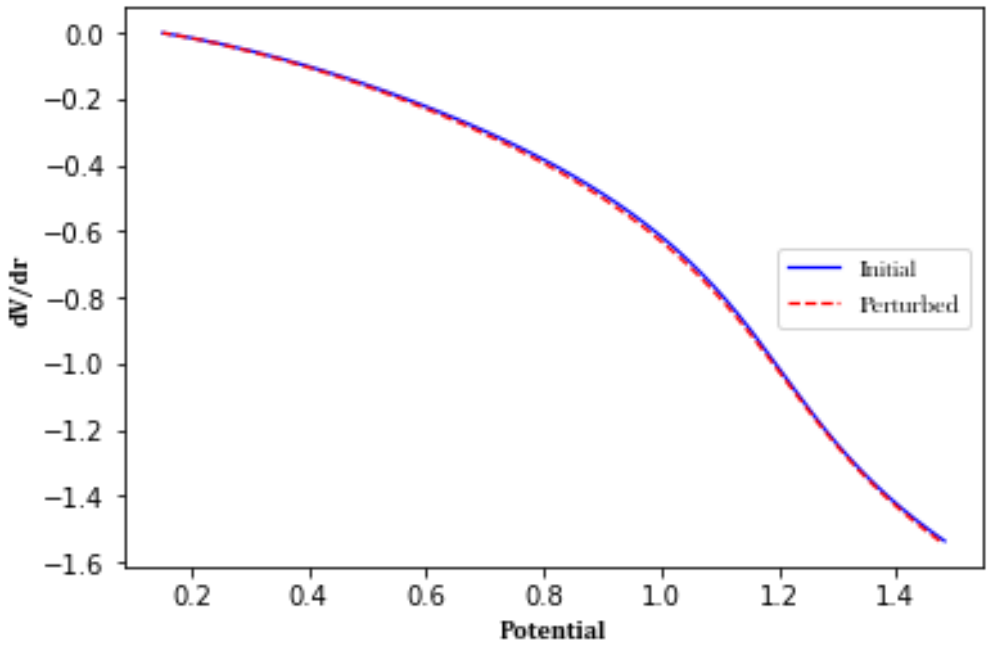


Fig 6.7: Stable differential effect of a 0.01 random perturbation configuration of α on the initial potential level

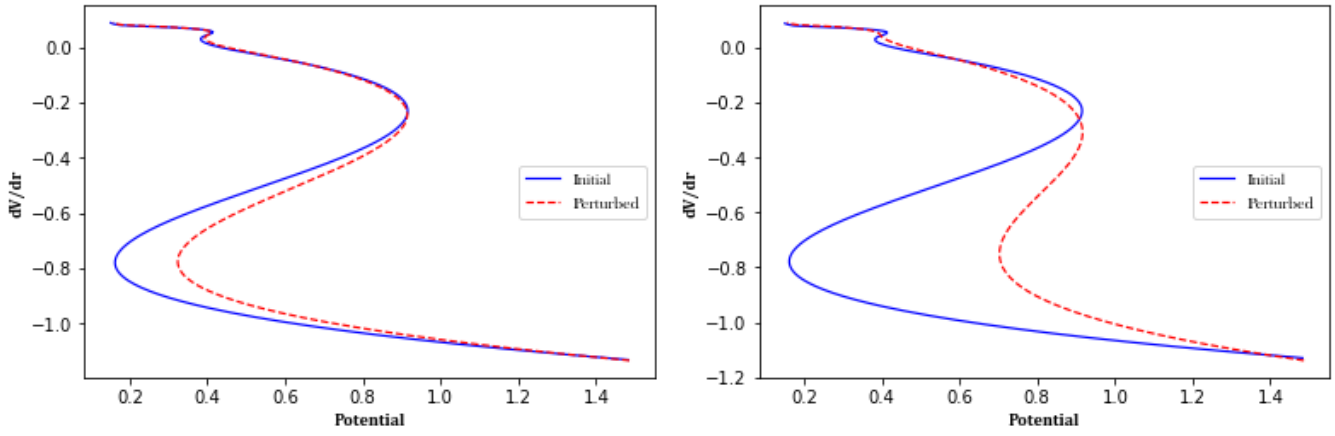


Fig 6.8 (a) and (b): Stochastic trends when α was increased to 0.5 and α was subjected to a 0.01 perturbation configuration

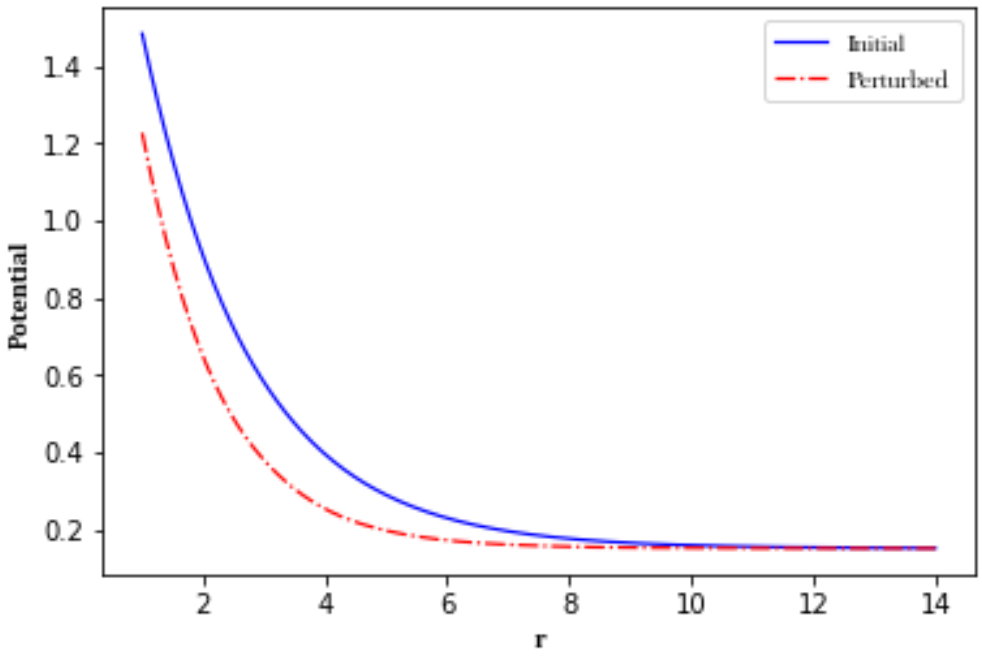


Figure 6.9: Variation of the potential levels as a function of r under a 0.4 perturbation configuration of α

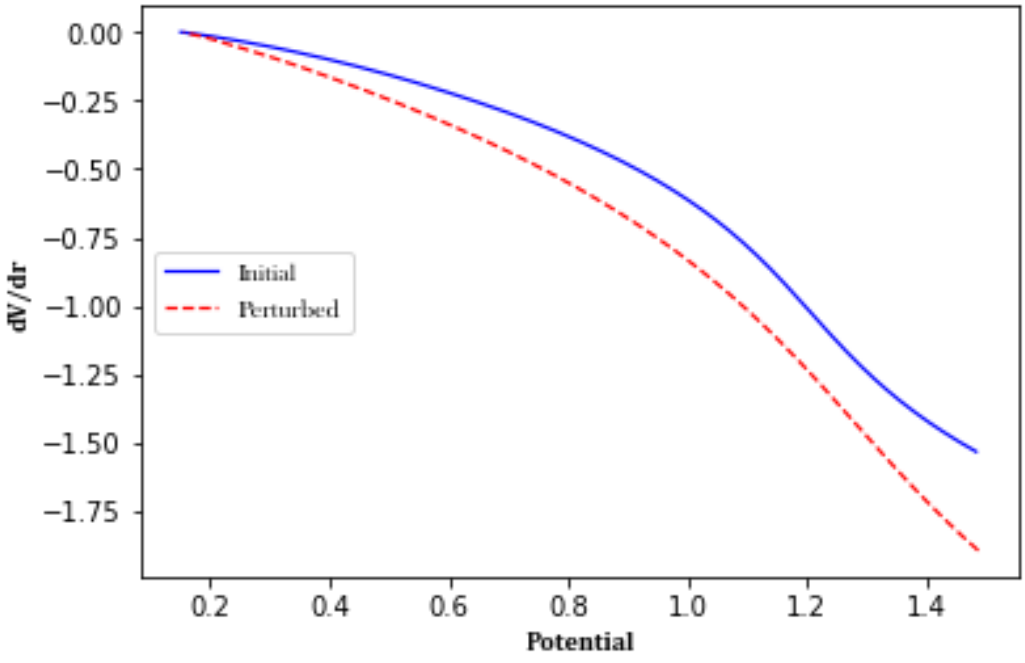


Fig 6.10: Stable differential effect of a 0.4 random perturbation configuration of α on the initial potential level.

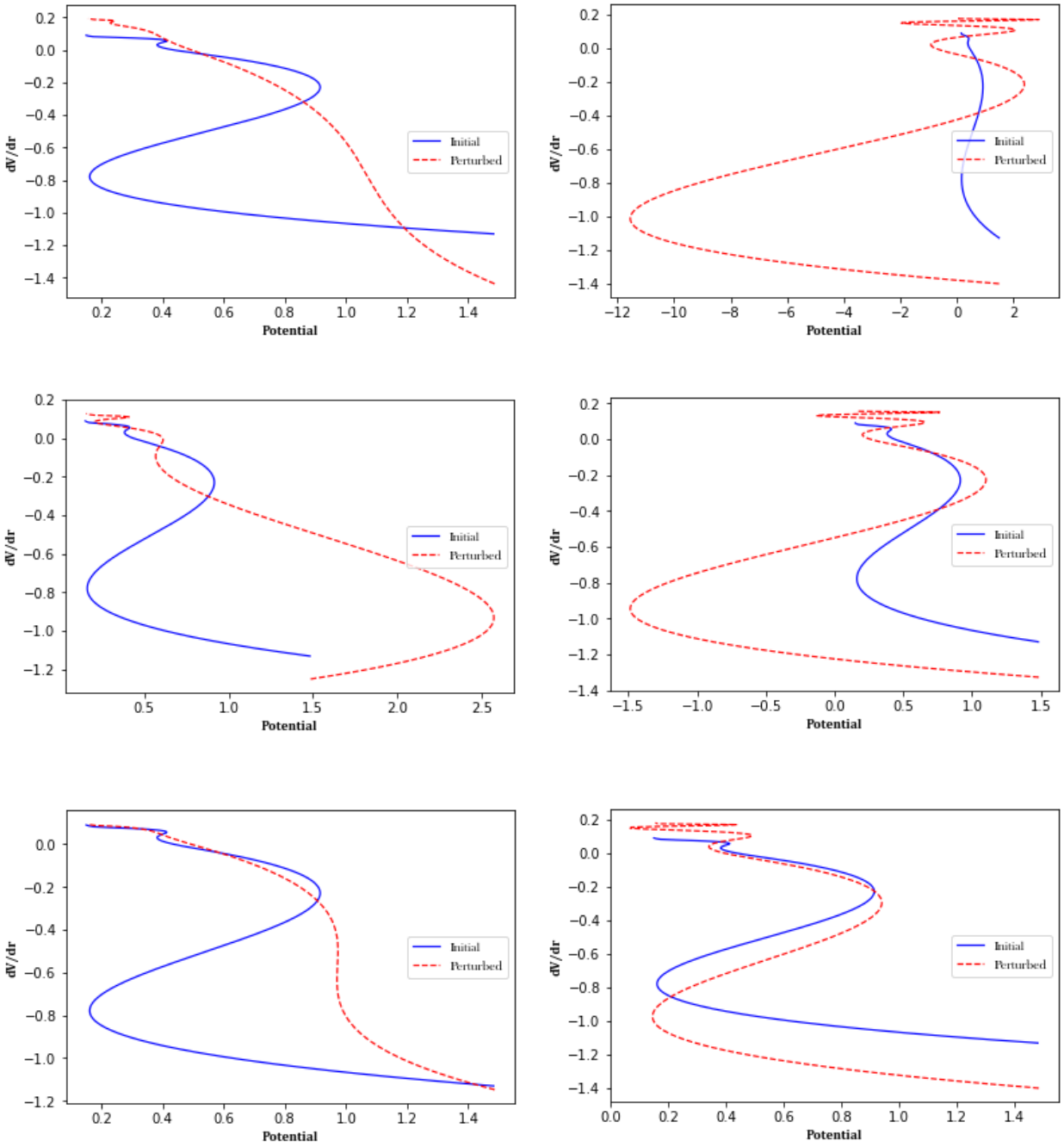


Fig 6.11 (a) - (f): Unstable stochastic trends when a was increased to 0.5 and α was subjected to a 0.4 perturbation configuration

From the plots, we see an agreement with our stability analysis in Section 3.2, where dV becomes zero at $V = a = 0.15$. This is also the same case when the value of a is increased to 0.5. Further, the plots demonstrate that the screening parameter α controls the shape of the potential energy curves, in agreement with theoretical literature. Indeed, the potential energy curves straighten out as the value of α increases.

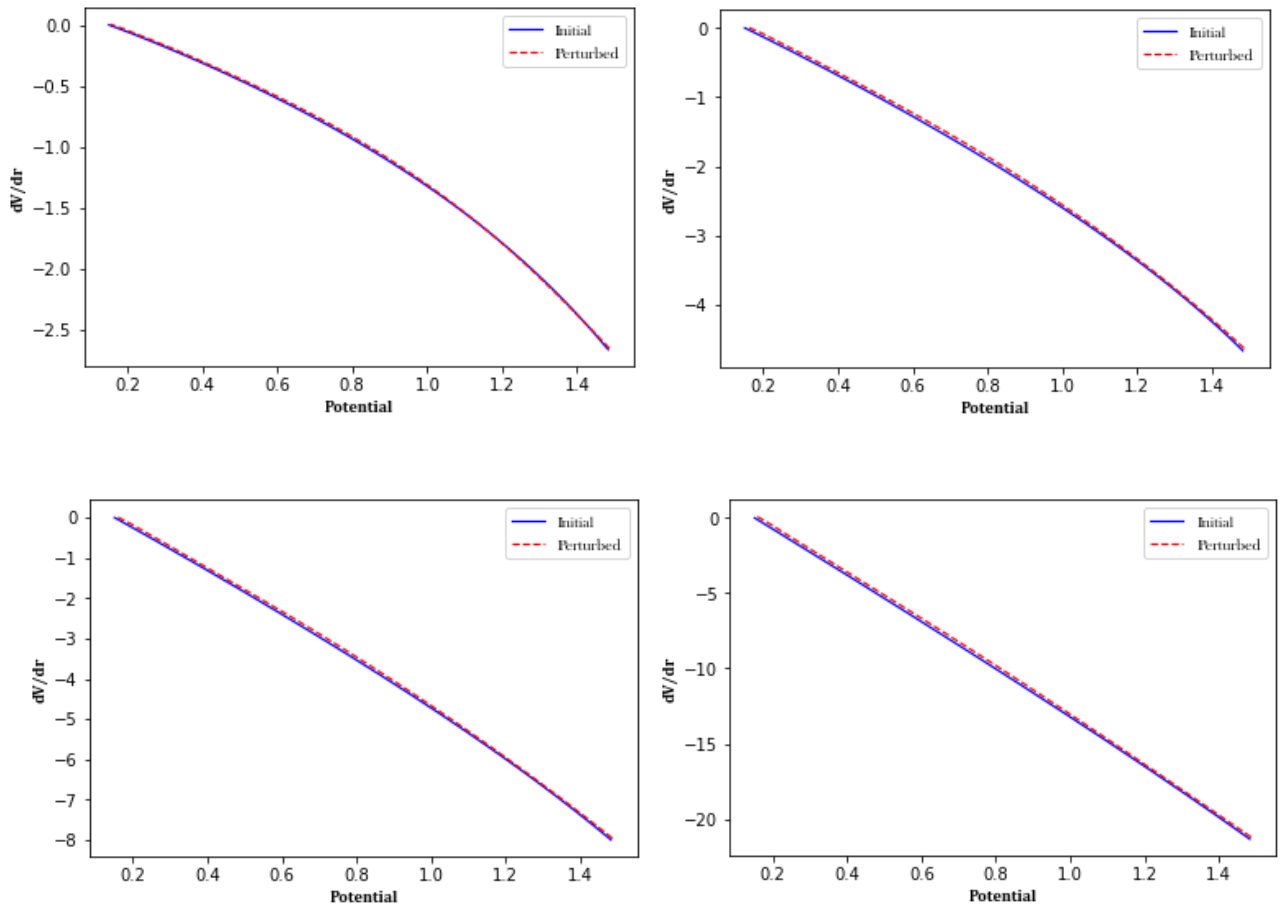


Fig 6.12 (a)-(d): Differential effects of arbitrary random perturbation configurations for initial values $\alpha = 1$, 2.5, 5, and 15 respectively.

7. CONCLUSIONS AND FURTHER RESEARCH

Our numerical simulations revealed that the potential strength a is increasingly sensitive to random perturbations, resulting in unstable fluctuations in the system's behaviour. The higher the value of a, the more periodic the system and the more unstable the fluctuations under perturbation. For smaller values of a, lower initial values of screening parameter α result in higher curvatures in the plots, and when perturbed, produce more stable fluctuations. However, the influence of α over the stability of fluctuations thins out inversely with a and the fluctuations become more unstable. Finally, in all configurations, as α increases, the potential energy curves straighten out irrespective of any perturbations in a or α. In general, variations in a have direct differential effects on the periodicity and stability of the system, while variations in α have direct effects on the shape of the curves.

Our findings in this study and the methods we employed can be extended to tackle the following research problems which we did not consider here:

- Differential effects of simultaneously varying the model parameters on the potential V.
- Numerical effects of varying the iteration intervals and range of initial conditions on V.

- Influence of computational time delays on the outcome of the numerical simulation.
- Error analysis of interacting solution trajectories to determine model accuracy.

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APPENDIX 1

A. MATLAB Codes for Numerical Integration

```
clear all
clc

function  dN = zion10(t,N)
dN = zeros(1,1);
a = 0.15;
alpha = 0.15;
r = 2.4;
dN(1) = (a-N(1))*(alpha+(1/r))

function  dN=zion11(t,N)
dN = zeros(1,1);
a = 0.15+0.01*rand(1);
alpha = 0.15;
r = 2.4;
dN(1)=(a-N(1))*(alpha+(1/r))

function  dN=zion12(t,N)
```

```
dN=zeros(1,1);
a=0.15+0.4*rand(1);
alpha=0.15;
r=2.4;
dN(1)=(a-N(1))*(alpha+(1/r)
```

```
function  dN=zion13(t,N)
dN=zeros(1,1);
a=0.15;
alpha=0.15+0.01*rand(1);
r=2.4;
dN(1)=(a-N(1))*(alpha+(1/r))
```

```
function  dN=zion14(t,N)
dN=zeros(1,1);
a=0.15;
alpha=0.15+0.4*rand(1);
r=2.4;
dN(1)=(a-N(1))*(alpha+(1/r))
```

Configuration 1 Simulation

```
t = 0:1:14
[t    Y] = ode45(@zion10,  [t], [2.5],'reltol=0.001')
[t    Y1] = ode45(@zion11,  [t], [2.5],'reltol=0.001')
E1 = [(Y1-Y)./Y]*100
ANS = [t      Y      Y1         E1]
```

Configuration 2 Simulation

```
t = 0:1:14
[t    Y] = ode45(@zion10,  [t], [2.5],'reltol=0.001')
[t    Y1] = ode45(@zion12,  [t], [2.5],'reltol=0.001')
E1 = [(Y1-Y)./Y]*100
ANS = [t      Y      Y1         E1]
```

Configuration 3 Simulation

```
t = 0:1:14
[t    Y] = ode45(@zion10,  [t], [2.5],'reltol=0.001')
```

```
[t    Y1] = ode45(@zion13,  [t], [2.5],'reltol=0.001')
E1 = [(Y1-Y)./Y]*100
ANS = [t      Y      Y1         E1]
```

Configuration 4 Simulation

```
t = 0:1:14
[t    Y] = ode45(@zion10,  [t], [2.5],'reltol=0.001')
[t    Y1] = ode45(@zion14,  [t], [2.5],'reltol=0.001')
E1 = [(Y1-Y)./Y]*100
ANS = [t      Y      Y1         E1]
K=Y-Y1
```

B. Python Codes for Data Visualisation

```
# Load dependencies
import pandas as pd
import numpy as np
from random import *
from scipy.interpolate import make_interp_spline,BSpline
import matplotlib.pyplot as plt
%matplotlib inline
```

Configuration 1: Low Perturbation of a on V

```
# Import data for Case 1
case1=pd.read_csv('config1.csv', header = None)

#Drop missing values
case1.drop([0],inplace = True)
case1.dropna(axis=1,inplace = True)

# Plot r against initial and modified potentials
r = np.linspace(case1[1].min(),case1[1].max(),300)
spline1 = make_interp_spline(case1[1],case1[2],k=3)
spline2 = make_interp_spline(case1[1],case1[3],k=3)
V1 = spline1(r)
V2 = spline2(r)
```

```
plt.plot(r,V1,'b',r,V2,'r-.',linewidth=1.2)
l = plt.legend(['Initial','Perturbed'],loc=9)
plt.setp(l.texts, family = 'Baskerville Old Face')
plt.xlabel('r',fontname = 'Cambria')
plt.ylabel('Potential', fontname = 'Cambria')

a = 0.15
alpha = 0.15
dV = (a-case1[2])*(alpha+1/case1[1])
dV1 = np.linspace(dV.min(),dV.max(),300)
spline1 = make_interp_spline(dV.sort_values(),case1[2],k=3)
V1smooth = spline1(dV1)
a_mod = 0.15 + 0.01*random()
dVnew = (a_mod-case1[2])*(alpha+1/case1[1])
dV2 = np.linspace(dVnew.min(),dVnew.max(),300)
spline2 = make_interp_spline(dVnew.sort_values(),case1[3],k=3)
V2smooth = spline2(dV2)
plt.plot(V1smooth,dV1,'b',V2smooth,dV2,'r--',linewidth=1.2)
l = plt.legend(['Initial','Perturbed'],loc=6)
plt.setp(l.texts, family = 'Baskerville Old Face')
plt.xlabel('Potential',fontname = 'Cambria')
plt.ylabel('dV/dr', fontname = 'Cambria')

a = 0.5
alpha = 0.15
dV = (a-case1[2])*(alpha+1/case1[1])
dV1 = np.linspace(dV.min(),dV.max(),300)
spline1 = make_interp_spline(dV.sort_values(),case1[2],k=3)
V1smooth = spline1(dV1)
a_mod = 0.5 + 0.01*random()
dVnew = (a_mod-case1[2])*(alpha+1/case1[1])
dV2 = np.linspace(dVnew.min(),dVnew.max(),300)
spline2 = make_interp_spline(dVnew.sort_values(),case1[3],k=3)
V2smooth = spline2(dV2)
plt.plot(V1smooth,dV1,'b',V2smooth,dV2,'r--',linewidth=1.2)
```

```
l = plt.legend(['Initial','Perturbed'],loc=7)
plt.setp(l.texts, family = 'Baskerville Old Face')
plt.xlabel('Potential',fontname = 'Cambria')
plt.ylabel('dV/dr', fontname = 'Cambria')
```

Configuration 2: High Perturbation of $\boldsymbol{a}$ on $\boldsymbol{V}$

```
# Import data for Case 2
case2 = pd.read_csv('config2.csv', header = None)

#Drop missing values
case2.drop([0],inplace = True)
case2.dropna(axis=1,inplace = True)

# Plot r against initial and modified potentials
r = np.linspace(case2[1].min(),case2[1].max(),300)
spline1 = make_interp_spline(case2[1],case2[2],k=3)
spline2 = make_interp_spline(case2[1],case2[3],k=3)
V1 = spline1(r)
V2 = spline2(r)
plt.plot(r,V1,'b',r,V2,'r--',linewidth=1.2)
l = plt.legend(['Initial','Perturbed'],loc=9)
plt.setp(l.texts, family = 'Baskerville Old Face')
plt.xlabel('r',fontname = 'Cambria')
plt.ylabel('Potential', fontname = 'Cambria')

a = 0.15
alpha = 0.15
dV = (a-case1[2])*(alpha+1/case1[1])
dV1 = np.linspace(dV.min(),dV.max(),300)
spline1 = make_interp_spline(dV.sort_values(),case1[2],k=3)
V1smooth = spline1(dV1)
a_mod = 0.15 + 0.4*random()
dVnew = (a_mod-case1[2])*(alpha+1/case1[1])
dV2 = np.linspace(dVnew.min(),dVnew.max(),300)
spline2 = make_interp_spline(dVnew.sort_values(),case1[3],k=3)
```

```
V2smooth = spline2(dV2)
plt.plot(V1smooth,dV1,'b',V2smooth,dV2,'r--',linewidth=1.2)
l = plt.legend(['Initial','Perturbed'],loc=6)
plt.setp(l.texts, family = 'Baskerville Old Face')
plt.xlabel('Potential',fontname = 'Cambria')
plt.ylabel('dV/dr', fontname = 'Cambria')

a = 0.5
alpha = 0.15
dV = (a-case1[2])*(alpha+1/case1[1])
dV1 = np.linspace(dV.min(),dV.max(),300)
spline1 = make_interp_spline(dV.sort_values(),case1[2],k=3)
V1smooth = spline1(dV1)
a_mod = 0.5 + 0.4*random()
dVnew = (a_mod-case1[2])*(alpha+1/case1[1])
dV2 = np.linspace(dVnew.min(),dVnew.max(),300)
spline2 = make_interp_spline(dVnew.sort_values(),case1[3],k=3)
V2smooth = spline2(dV2)
plt.plot(V1smooth,dV1,'b',V2smooth,dV2,'r--',linewidth=1.2)
l = plt.legend(['Initial','Perturbed'],loc=9)
plt.setp(l.texts, family = 'Baskerville Old Face')
plt.xlabel('Potential',fontname = 'Cambria')
plt.ylabel('dV/dr', fontname = 'Cambria')
```

Configuration 3: Low Perturbation of α on V

```
# Import data for Case 3
case3=pd.read_csv('config3.csv', header = None)

#Drop missing values
case3.drop([0],inplace = True)
case3.dropna(axis=1,inplace = True)

#Plot r against initial and modified potentials
r = np.linspace(case3[1].min(),case3[1].max(),300)
spline1 = make_interp_spline(case3[1],case3[2],k=3)
```

```
spline2 = make_interp_spline(case3[1],case3[3],k=3)
V1 = spline1(r)
V2 = spline2(r)
plt.plot(r,V1,'b',r,V2,'r--',linewidth=1.2)
l = plt.legend(['Initial','Perturbed'],loc=9)
plt.setp(l.texts, family = 'Baskerville Old Face')
plt.xlabel('r',fontname = 'Cambria')
plt.ylabel('Potential', fontname = 'Cambria')

a = 0.15
alpha = 0.15
dV = (a-case1[2])*(alpha+1/case1[1])
dV1 = np.linspace(dV.min(),dV.max(),300)
spline1 = make_interp_spline(dV.sort_values(),case1[2],k=3)
V1smooth = spline1(dV1)
alpha_mod = 0.15 + 0.01*random()
dVnew = (a-case1[2])*(alpha_mod+1/case1[1])
dV2 = np.linspace(dVnew.min(),dVnew.max(),300)
spline2 = make_interp_spline(dVnew.sort_values(),case1[3],k=3)
V2smooth = spline2(dV2)
plt.plot(V1smooth,dV1,'b',V2smooth,dV2,'r--',linewidth=1.2)
l = plt.legend(['Initial','Perturbed'],loc=6)
plt.setp(l.texts, family = 'Baskerville Old Face')
plt.xlabel('Potential',fontname = 'Cambria')
plt.ylabel('dV/dr', fontname = 'Cambria')

a = 0.5
alpha = 0.15
dV = (a-case1[2])*(alpha+1/case1[1])
dV1 = np.linspace(dV.min(),dV.max(),300)
spline1 = make_interp_spline(dV.sort_values(),case1[2],k=3)
V1smooth = spline1(dV1)
alpha_mod = 0.15 + 0.01*random()
dVnew = (a-case1[2])*(alpha_mod+1/case1[1])
dV2 = np.linspace(dVnew.min(),dVnew.max(),300)
```

```
spline2 = make_interp_spline(dVnew.sort_values(),case1[3],k=3)
V2smooth = spline2(dV2)
plt.plot(V1smooth,dV1,'b',V2smooth,dV2,'r--',linewidth=1.2)
l = plt.legend(['Initial','Perturbed'],loc=7)
plt.setp(l.texts, family = 'Baskerville Old Face')
plt.xlabel('Potential',fontname = 'Cambria')
plt.ylabel('dV/dr', fontname = 'Cambria')
```

Configuration 4: High Perturbation of α on V

```
#Import data for Case 4
case4 = pd.read_csv('config4.csv', header = None)

#Drop missing values
case4.drop([0],inplace = True)
case4.dropna(axis=1,inplace = True)

# Plot r against initial and modified potentials
r = np.linspace(case4[1].min(),case4[1].max(),300)
spline1 = make_interp_spline(case4[1],case4[2],k=3)
spline2 = make_interp_spline(case4[1],case4[3],k=3)
V1 = spline1(r)
V2 = spline2(r)
plt.plot(r,V1,'b',r,V2,'r-.',linewidth=1.2)
l = plt.legend(['Initial','Perturbed'],loc=1)
plt.setp(l.texts, family = 'Baskerville Old Face')
plt.xlabel('r',fontname = 'Cambria')
plt.ylabel('Potential', fontname = 'Cambria')

a = 0.15
alpha = 0.15
dV = (a-case1[2])*(alpha+1/case1[1])
dV1 = np.linspace(dV.min(),dV.max(),300)
spline1 = make_interp_spline(dV.sort_values(),case1[2],k=3)
V1smooth = spline1(dV1)
alpha_mod = 0.15 + 0.4*random()
```

```
dVnew = (a-case1[2])*(alpha_mod+1/case1[1])
dV2 = np.linspace(dVnew.min(),dVnew.max(),300)
spline2 = make_interp_spline(dVnew.sort_values(),case1[3],k=3)
V2smooth = spline2(dV2)
plt.plot(V1smooth,dV1,'b',V2smooth,dV2,'r--',linewidth=1.2)
l = plt.legend(['Initial','Perturbed'],loc=6)
plt.setp(l.texts, family = 'Baskerville Old Face')
plt.xlabel('Potential',fontname = 'Cambria')
plt.ylabel('dV/dr', fontname = 'Cambria')

a = 0.5
alpha = 0.15
dV = (a-case1[2])*(alpha+1/case1[1])
dV1 = np.linspace(dV.min(),dV.max(),300)
spline1 = make_interp_spline(dV.sort_values(),case1[2],k=3)
V1smooth = spline1(dV1)
alpha_mod = 0.15 + 0.4*random()
dVnew = (a-case1[2])*(alpha_mod+1/case1[1])
dV2 = np.linspace(dVnew.min(),dVnew.max(),300)
spline2 = make_interp_spline(dVnew.sort_values(),case1[3],k=3)
V2smooth = spline2(dV2)
plt.plot(V1smooth,dV1,'b',V2smooth,dV2,'r--',linewidth=1.2)
l = plt.legend(['Initial','Perturbed'],loc=7)
plt.setp(l.texts, family = 'Baskerville Old Face')
plt.xlabel('Potential',fontname = 'Cambria')
plt.ylabel('dV/dr', fontname = 'Cambria')
```