Scattering Simulation under Several Classical Central Force Potential

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Abstract: Scattering differential section for several central force potentials has been simulated in a numerical way in this paper. Here presents the introduction to the theory of scattering, the algorithm structure of numerical simulation, and finally the simulation results and discussion. This paper is a typical example of comprehensive utilization of numerical calculus methods.

Key Words: numerical simulation, scattering differential section, central force potential

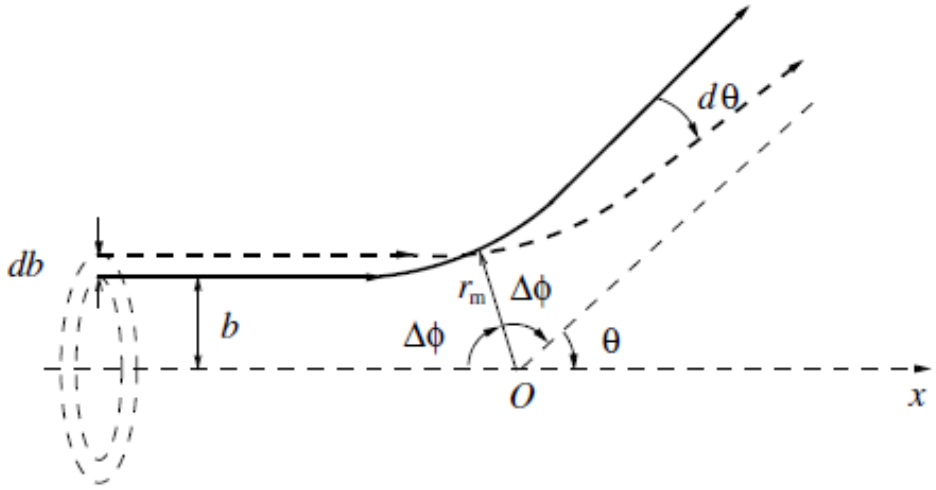
1 Introduction to the Theory of Scattering

1.1 General Theory for two-body system[1,2]

Scattering is a very common and important phenomenon in classical physics, for it can take place either in an astronomical scale or in a microscopic scale. In general, scattering is a many-body problem, which can seldom be solved analytically.

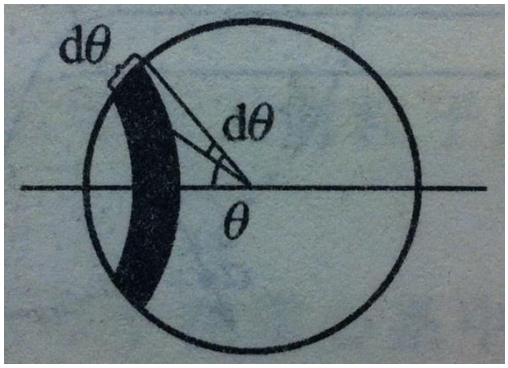
To simplify the discussion involved here, I shall limit the discussion to two-body situation only in this paper. In addition, we will assume the central force field exerting on two interacting particles is spherically symmetric. Thus, we have the total angular momentum conservation and energy conservation for the system.

A particle with mass *m* in a central potential *V(r)* comes in from the left with an impact parameter *b*. *Impact parameter* is the minimal perpendicular distance between the particle and the extrapolated line started from the center of spherically symmetric potential.



(cited from [1])

The differential cross section,$\sigma(\theta)$, describes the probability of a particle's being found in the solid angle element $d\Omega$ at the deflection angle θ, where $d\Omega = \frac{2\pi r sin\theta \cdot r d\theta}{r^2}$



(cited from [2])

If the particles are coming in with a flux density *I* (number of particles per unit cross-sectional area per unit time), the number of particles per unit time within the range of *db* of the impact parameter *b* is $I \cdot (2\pi b \cdot db)$. Because all the incoming particles in this area will go out in the solid angle element $d\Omega$ with the probability $\sigma(\theta)$, we have

$$\sigma(\theta) = \frac{b}{\sin\theta}\left|\frac{db}{d\theta}\right|$$

1.2 Algorithm Structure and Numerical Simulation Scheme

Basic idea: When we have a particle coming in with *an initial impact parameter b,* the particle will have a *certain minimal distance, r_m, to the center* of potential during the whole process. Then there comes *a certain angle* θ in which the *particle leaves.*

The basic procedure is taken as the follows:

①Starting known conditions should be:

A given set of *(impact parameter b, energy of incident particle E)*

⇩

②The *minimum distance* to the center r_m

⇩

③*The angle* θ in which the particle leaves

⇩

④A given b generates a certain θ. Pack them together in corresponding order.

I shall not derive all the analytical results here, since what we only concern here is numerical simulation. All the results can be deducted from two conservation

relations quite straightforwardly (Conservation of angular momentum $l = mr^2\dot{\phi}$ *and* conservation of energy $E = \frac{m}{2}\left(\dot{r}^2 + r^2\dot{\phi}^2\right) + V(r)$).

The corresponding numerical analysis procedure is shown as following:

①*Starting known conditions* should be:

A given set of *(impact parameter b, energy of incident particle E)*

②The *minimum distance* to the center r_m is given by the equation

$$1 - \frac{b^2}{{r_m}^2} - \frac{V(r_m)}{E} = 0$$

I shall solve this equation by *secant method* (in which *Lagrange interpolation* will also be used).

③*The angle* θ in which the particle leaves is given by the integral

$$\theta = 2b\left[\int_b^\infty \frac{dr}{r^2\sqrt{1-\left(\frac{b}{r}\right)^2}} - \int_{r_m}^\infty \frac{dr}{r^2\sqrt{1-\left(\frac{b}{r}\right)^2 - \frac{V(r)}{E}}}\right]$$

I shall evaluate this integral by *Simpson method*.

Explanation to the first term: It's obvious that its *accurate value is just* π. However, it should be noticed that both integrals are diverging at the very beginning of integration process, that is, when *r* is near *b* or r_m respectively for both integrals. Dividing the integrating process into two parts artificially will cancel the rolling errors originated from the initial 'diverging' situation, because this inevitable circumstance influences both integrals.

It's worthwhile to point out that $\Delta\phi$ is obtained after direct operation of integral to

$$\frac{d\phi}{dr} = \pm\frac{b}{r^2\sqrt{1-\left(\frac{b}{r}\right)^2 - \frac{V(r)}{E}}}$$

and notice $\theta = \pi - 2\Delta\phi$.

It is vital for us to decide when the plus sigh should be adopted or the minus should. From the point of view of the physical process, in the first half process the minus sigh must be adopted and in the second half process plus sigh is the correct on to describe the real physical process.

④A given b generates a certain θ. Pack them together in corresponding order.

I shall evaluate the derivative $\frac{db}{d\theta}$ by *the three-point formula*.

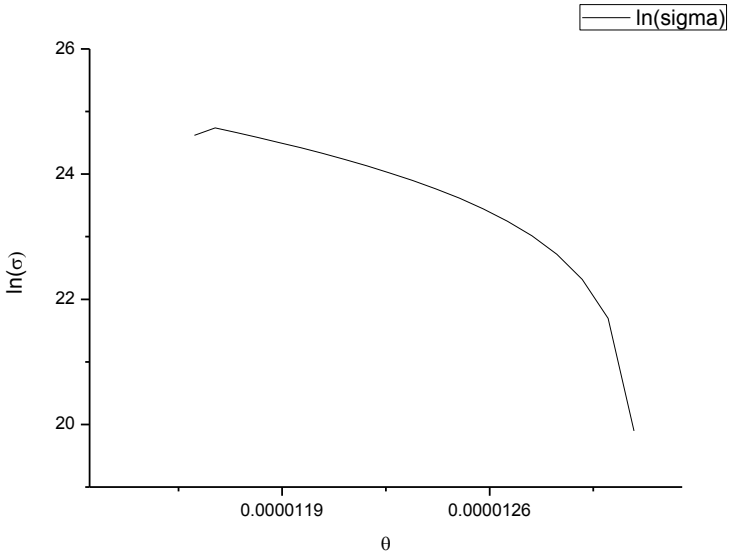
2 Simulation results

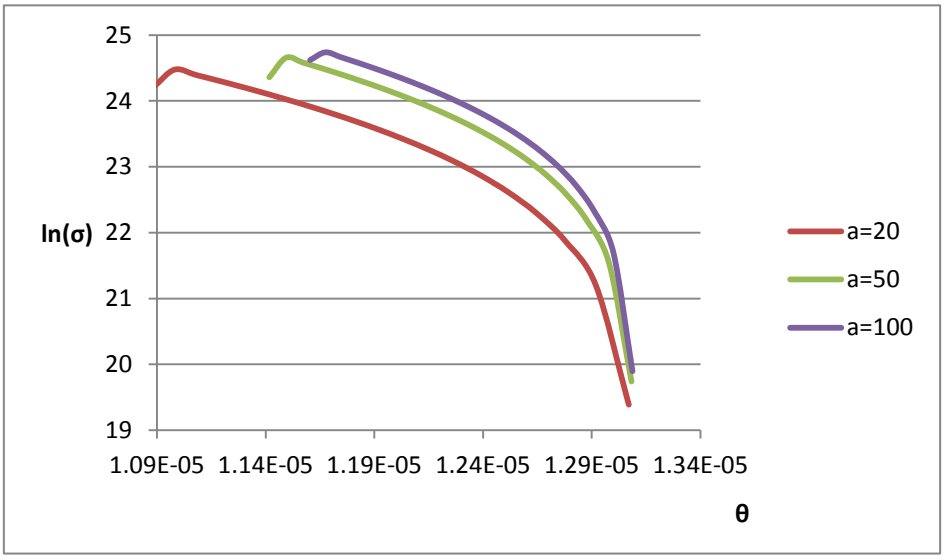
2.1 Yukuwa Potential $V(r) = \frac{\kappa}{r} e^{-\frac{r}{a}}$

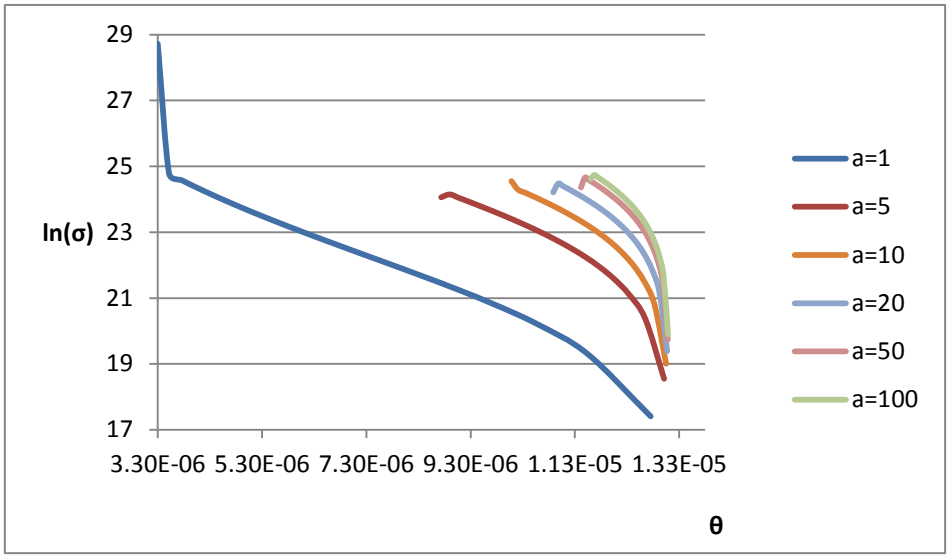
Potential parameters: $\kappa = 1, a = 100$

Incident parameters: E=10^5

Integral parameters: h=10^{-5}, double Simpson Integral



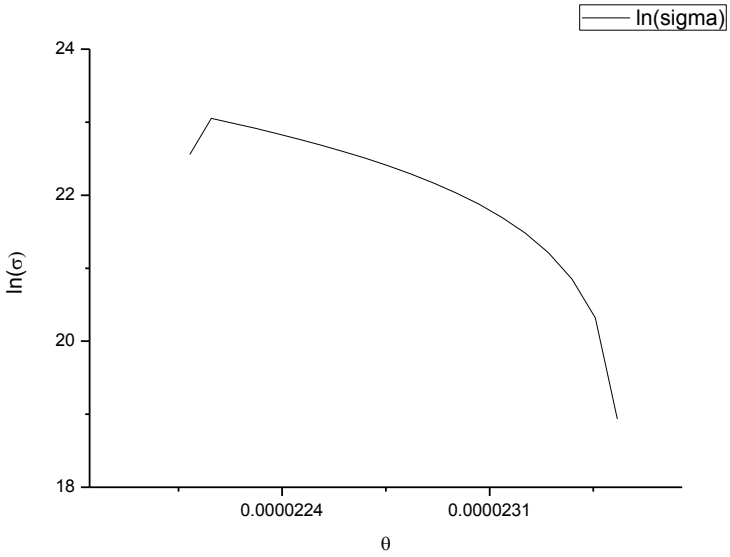




The above graph conveys that when *a* becomes larger, possibility distribution has been shifted to the 'right direction' along θ axis. In other words, for a given small scattering angle, it seems I could find more particles when *a* is large (less scattered).

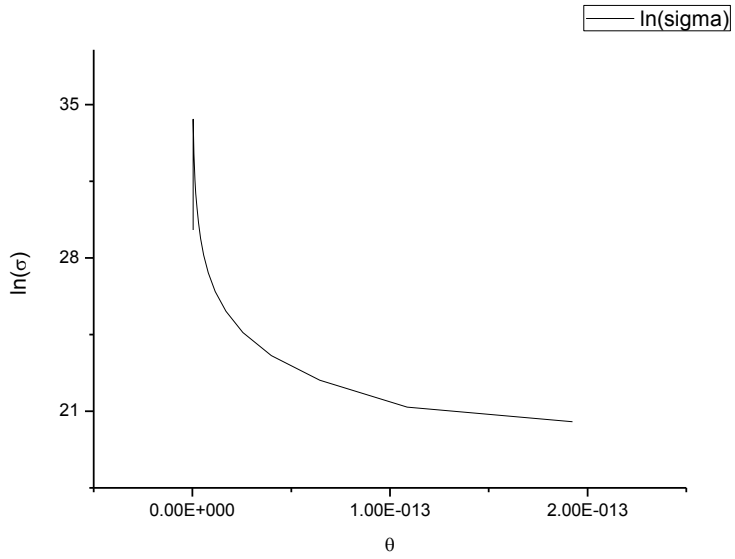
2.2 Coulomb Potential $V(r) = \frac{1}{4\pi\epsilon_0}\frac{1}{r}$

Incidence parameters: $E = 5 \times 10^{14}$,
Integral Parameters: h=10^{-5}, double Simpson Integral



2.3 Leonnard-Jones Potential $V(r) = 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$

Potential parameters for water molecules: $\epsilon = 1.8 \times 10^{-21}, \sigma = 0.32 \times 10^{-9}$
Tested when b_0=10^{-8}, db=10^{-9}, incident energy E set as 10^{-20}(>> Potential Energy ~10^{-27}, around 7 scales larger)
Integral parameters set as h=10^{-4}, n=10^{7}, double Simpson integral



3 Brief Explanation to the physical meaning of simulation graph

In the first section, I have mentioned that the differential cross section tells the possibility at which the leaving particles are found at a specific angle θ.

What we can expect is that when the total mechanical energy is large, the particle is high likely to overcome the attractive or compelling force and to leave the area where the potential functions effectively in a short time. Therefore, the divergent angle should be pretty small.

What is more important, with a fixed incident energy *E*, we can predict that, when a group of particles shooting towards and crossing the potential area, it is harder to find outgoing particles with a significantly large distorted angle for its movement than those with a small distorted angle. All reasonable plots should depict such an overall tendency that as the distorted angle θ *is increasing*, the possibility to find outgoing particles, that is, the differential cross section σ, presents a *decreasing* tendency. In addition, the reasonable value of ln(σ) should be positive, s

However, I cannot specify the appearance of the curve, or more mathematically presented, the function characteristics of $\sigma = \sigma(\theta)$. Whether the behavior of the curve will be distorted or not largely depends on the quality of numerical calculation, which I shall discuss in the following section.

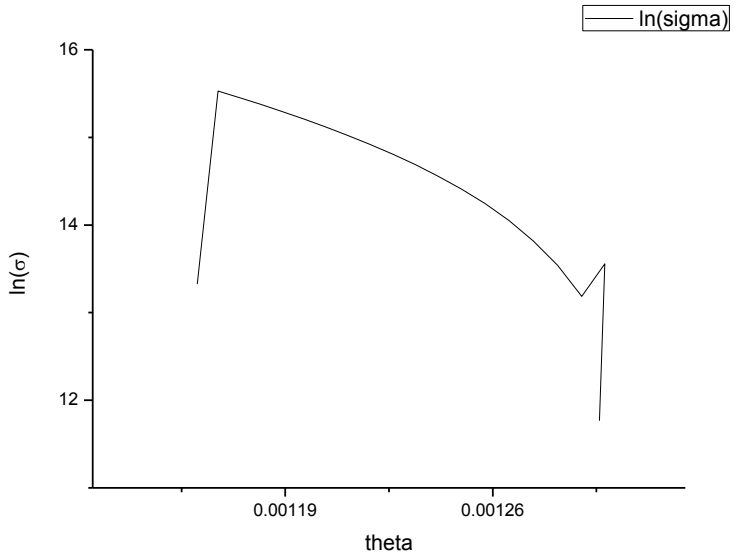
4 Discussion about *NUMERICAL ERRORS*

This part is probably the most interesting part!

4.1 The influence of the initial parameters

The smaller the incident energy is, the larger the numerical error will be.

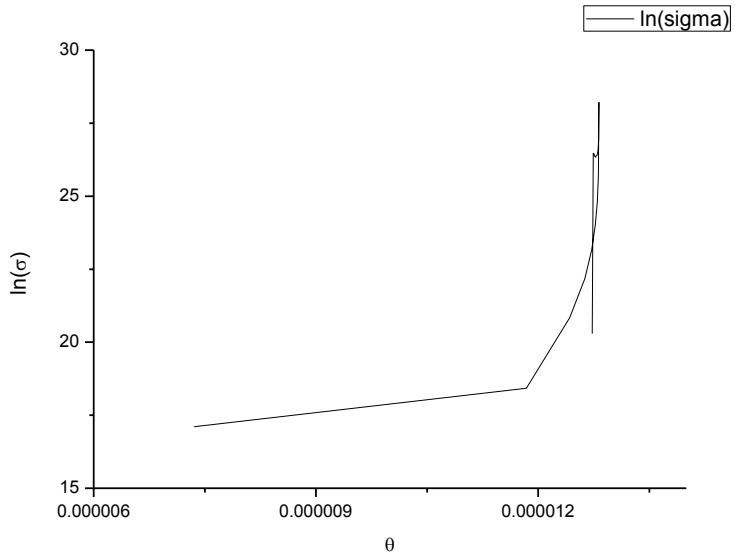
Yukawa Potential when $h=10^{-5}$, $E=10^{3}$



It is much less smooth than the result we get when we set the incident energy E as 10^5. It tells us that the Simpson integration method is still too rough to depict a relatively small system behavior shift, i.e. when the energy is altered.

4.2 The influence of the *interval of arguments* in numerical integration '*h*'

Yukawa Potential when h=0.01, E=10^5, double Simpson Integral



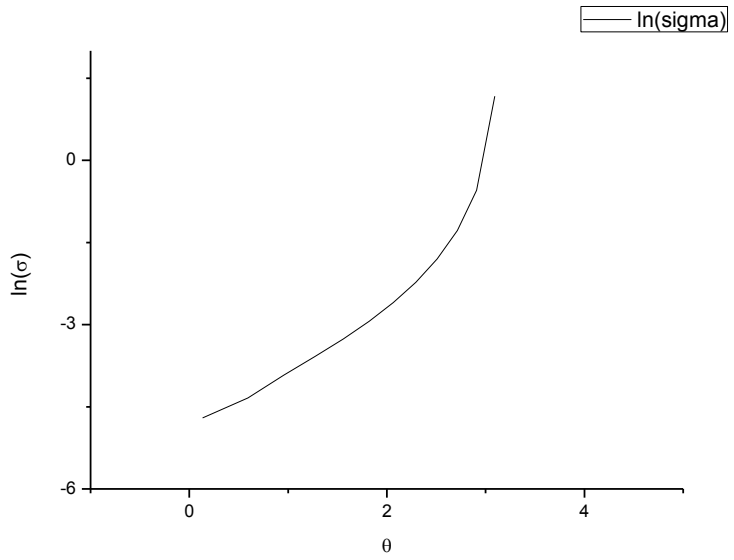
Now the problem is extremely overwhelming, since the whole tendency is completely up-side-down switch---an *INCREASING* tendency. This is definitely not acceptable from the point of view of physics.

In the beginning stage of my work to this paper, I always got this unphysical result, which was quite frustrating to me. It shows that how insufficient the accuracy of Simpson Integration is.

4.3 Always providing physically reasonable initial conditions

h=10^{-5} for Coulomb Potential when E=1

V~10^{14}, now E<<V, implying E_k<0!!!



4.4 The influence of 'π'

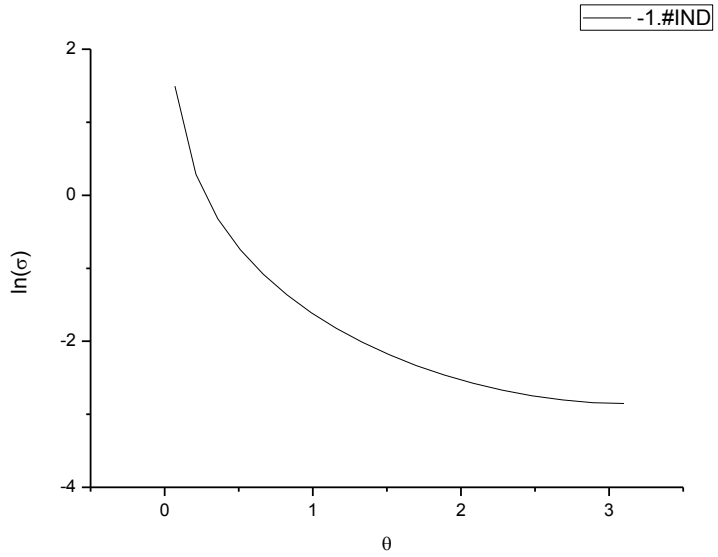
Only one Simpson Integration conducted, the first integration is directly substituted by its analytical value π

Yukawa Potential:

Potential parameters: $\kappa = 1, a = 100$

Incidence parameters: E=10^5

Integral parameters: h=10^{-5}, *SINGLE* Simpson Integral

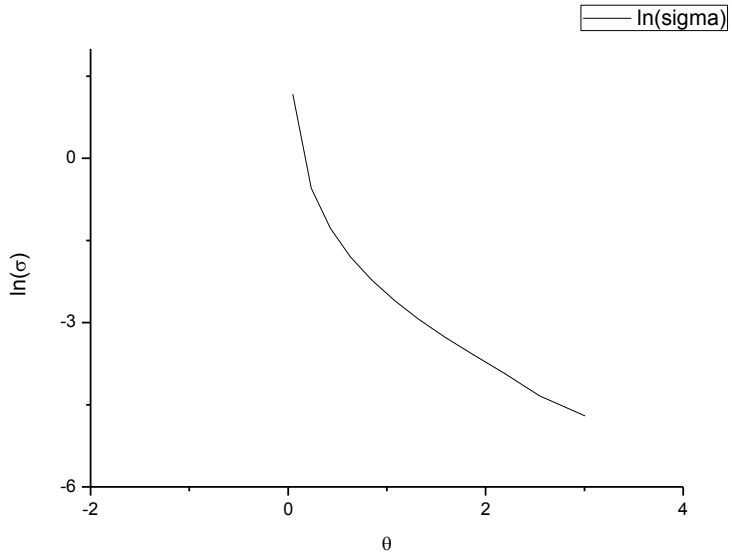


Coulomb Potential:

Potential parameters: $\kappa = 1, a = 100$

Incidence parameters: E=5×10^{14}

Integral parameters: h=10^{-5}, *SINGLE* Simpson Integral



It is undeniable that the line shape presented is terrifically beautiful! What is more important, it correctly shows the real line shape of the analytical differential cross section $\sigma = \sigma(\theta)$. What we sacrifice here is still '*physically accepted*'. The last 8 scattering angles θ of the Yukawa potential is *SMALLER* than 0, which is definitely wrong in physics (the particle shot from the upper half space and leaving in the lower half space with a scattering angle larger than 180° !!!) For Coulomb potential there are also 8 final scattering angles θ are smaller than 0!!

The following data is the obtained using SINGLE Simpson integration for Yukawa Potential.

θ	ln(σ)	θ	ln(σ)
-1.19981	-1.#IND	0.42811	-1.28165
-1.06256	-1.#IND	0.63267	-1.80216
-0.92071	-1.#IND	0.8485	-2.22642
-0.77396	-1.#IND	1.0773	-2.5977
-0.62194	-1.#IND	1.32133	-2.93788
-0.46425	-1.#IND	1.58375	-3.26147
-0.30044	-1.#IND	1.86923	-3.58205
-0.12998	-1.#IND	2.1855	-3.92014
0.04776	1.1716	2.54796	-4.33836
0.2335	-0.54559	3.00693	-4.70303

Table 1 Data of Single Simpson Integral for Yukawa Potential

Here presents a *tradeoff* in front of us:

A Physically Correct Simulation with Terrible Line Shape

VS.

A Beautiful Line Shape (probably the same as the analytical one) with *Wrong*

Physical Meaning.

5 Conclusion

Scattering processes with respect to three central potentials have been simulated in this paper. Possible numerical errors have also been thoroughly discussed. I believe when a better *numerical integration* method is applied, the outcome will be much more plausible.

6 References

[1] Pang, Tao Introduction to Computational Physics

[2] Yang, Fujia Atomic Physics

7 Additional Notes on How to Use the Code

(1) You should set initial conditions in the beginning part of the code where many constants are defined.

(2) Choose Different Potentials: When you want to change to another potential function which you want to simulate, change the last argument in the program function *secant* and the function in the integrand, which have both been noted in the original code. The last argument is a pointer pointing to the called function.

(3) If you want to invalidate the first integral which has the certain value π, make the integration code part of *'g1'* to be notification and also choose the second output command of '*theta[i]*'.