A method to solve the inverse problem of elastic quantum collisions using Jost functions

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Abstract. The studies of the cross sections that originate from the collisions between particles are very important on quantum scattering theory because from them it is possible to calculate the properties of the interacting particles, but in several cases we do not know the potential that models the interaction or its shape is very complex. Although, it is possible to obtain the interaction potential using some approaches based on the inverse problem methodology, as of yet there is no analytical method that can be used for this purpose. In this work, a method to solve the inverse problem in elastic collisions is presented and has the advantage that it is only necessary to know the experimental data of the elastic differential cross section for a single energy value. We tested this method with great success in the process of colliding electrons with hydrogen atoms.

1. Introduction

The inverse problem is of fundamental importance in quantum scattering theory due to it permits to calculate the interaction potential between the particles of the system and in this way it is possible to study the properties that these particles have. The inverse problem was developed by Fröberg [1] and Hylleraas [2] to directly determine the scattering potential from the experimental data without prior knowledge of its analytical form. After that, Bargmann [3] discussed the ambiguity of his solutions and found a kind of equivalent potentials that have the same phase shifts and the same discrete spectrum. Levinson [4] showed that the existence of bound states is a reason for losing of uniqueness in the determination of the potential. The inverse problem was also studied by De Alfaro and Regge [5] and Newton [6] for a fixed energy value and an arbitrary angular momentum value.

The number of papers developed to solve the inverse problem for a fixed energy value is high, however, the procedures performed are very unstable with respect to small scattering angles and give rise an infinity set of equivalent solutions [7,8]. On the other hand, semi-classical approaches have also been used to calculate the scattering potential. Hoyt [9] was the first scientist who resolve the inverse problem for classical scattering for monotonous potentials, Hoyt’s approach is based on knowledge of the cross section for different energy values. While, Fisov [10] proposed a more convenient method that requires knowing the cross section for a single energy value. After that, many authors studied the inverse problem using classical and semi-classical approaches, these methods are more practical and Buck discussed them in detail [7,8].
It is necessary to mention that although these methods are formulated in a mathematical way that is elegant, their solutions and practical applications have a high difficulty, because these procedures require of the completeness of the experimental data, so much so, that the problem about the influence of the incompleteness of the information on the form of the solution is still open, on the other hand, we must solve integral equations that are very difficult and moreover, it is necessary to know additional information about the bound states to remove the uncertainty that is connected with obtaining families of equivalent potentials. One way to avoid these drawbacks is to use a semi-classical approach to calculate the potential, but the latter has the disadvantage that the method is not a fully quantum focusing.

In this work, a method is presented to solve the inverse problem, for its implementation it is necessary to use a semi-empirical potential that exploits the physical part of the problem, this method has the advantage that it is only necessary to know the experimental data of the differential cross section of a single energy value, moreover, it is a fully quantum approach where easy equations are solved; finally, we apply our method to calculate the scattering potential that models the collision of electrons by hydrogen atoms.

2. Methodology

The experimental quantities that are reported in the collision processes are known as cross sections, among them, the elastic differential cross section which is calculated using Equation (1) (see reference [11]),

\[
\frac{d\sigma(\theta)}{d\Omega} = \frac{1}{2ik} \sum_{L=0}^{\infty} (2L+1) (exp(2i\delta_L(k)) - 1) P_L(cos\theta)^2,
\]

where \( k \) is the wave number of the incident particle, \( L \) is the angular momentum, \( P_L \) are the Legendre polynomials and \( \delta_L(k) \) are the phase shifts that are the quantities that have physical interest because they have all the information about the collision process [11]. Theoretically, there are many methods to calculate phase shifts, among them, we can find approaches based on Jost functions as the one reported by the authors in reference [12] and it is shown here in Equation (2).

\[
f'_{L}(k,r) - \frac{U'(r)}{U(r)} + 2 \frac{h^+_L(kr)}{h^-_L(kr)} f_{L}(k,r) - U(r)f_{L}(k,r) = 0.
\]

In Equation (2), \( U(r) = 2mV(r)/\hbar^2 \) represents the interaction between an incident particle, which has angular momentum \( L \) and wave number \( k = 2mE/\hbar^2 \), with a target; \( r \) is the distance between the particles; \( h^+_L(kr) \) are the Riccati-Hankel functions and \( f_{L}(k,r) \) are named as the Jost solutions. The quotation marks mean to derive with respect to \( r \). It is possible to calculate the Jost functions \( (F_L(k)) \) by means of Equation (3) (see reference [11]), after that the Equation (2) is solved.

\[
f_L(k,r) \xrightarrow{r \rightarrow \infty} F_L(k),
\]

and finally the phase shifts are related to the Jost functions by means of Equation (4) (see reference [11]).

\[
F_L(k) = |F_L(k)| exp(-i\delta_L).
\]

The idea of our method is to obtain the phase shifts using Equation (1) when the experimental data of the elastic differential cross section \( d\sigma(\theta)/d\Omega \) are known for several values of the scattering angle \( (\theta) \), after that, we propose a semi-empirical potential that has settings parameters, with this we solve the Equation (2), then the Jost functions are calculated with
the Equation (3) and after that, we obtain the phase shifts using Equation (4). The phase shifts calculated in this way depend on the same parameters as the semi-empirical potential, therefore, it is possible to fit the potential parameters if we fit the phase shifts that were calculated in this way with those phase shifts that were found from the experimental data of the elastic differential cross section.

To carry out the above, we named as $(d\sigma(\theta_i)/d\Omega)_{ex}$ to the experimental data of the elastic differential cross section for a fixed energy value and for each $\theta_i$ angle, then the least squares method is used to fit the set of experimental values $(d\sigma(\theta_i)/d\Omega)_{ex}$ to the corresponding theoretical function (Equation (1)), in this point the phase shifts are taken like settings parameters and we have to minimize the Equation (5) (see reference [13]).

$$\sum_{\theta_i=1}^{N} (\Delta_i)^2, \quad (5)$$

where $N$ is the number of experimental data $(d\sigma(\theta_i)/d\Omega)_{ex}$ that are known and the $\Delta_i$ quantities represent the distance that there is between each experimental value $(d\sigma(\theta_i)/d\Omega)_{ex}$ and the corresponding value on the theoretical curve given by Equation (1), thus, the $\Delta_i$ quantities are calculated by means of Equation (6).

$$\Delta_i = (d\sigma(\theta_i)/d\Omega)_{ex} - d\sigma(\theta_i)/d\Omega. \quad (6)$$

The phase shifts that were calculated from the experimental data using the least square method are named $\delta_L$, as mentioned above, after calculating the phase shifts by fitting, we propose a semi-empirical potential that has settings parameters, i.e., $V = V(r, \alpha_1, \alpha_2,...)$ where $\alpha_i$ are the settings parameters and we use the Equation (2), Equation (3), and Equation (4) to obtain the phase shifts that depend on the $\alpha_i$ parameters, this is, $\delta_L(\alpha_1, \alpha_2,...)$, finally, the settings parameters are calculated from the roots of Equations (7).

$$\delta_L - \delta_L(\alpha_1, \alpha_2,...) = 0. \quad (7)$$

3. Results and discussion

Now, we test the method proposed in this paper, modeling the scattering process of electrons by hydrogen atoms when the energy of the system is $10\, eV$. In the literature there is few information about the experimental data of the elastic differential cross section of this system, but in references [12, 14] we can find the static potential of this collision, then we used it to calculate the values of the elastic differential cross section using the Equation (1) and we took them like $(d\sigma(\theta_i)/d\Omega)_{ex}$.

In Table 1 the values of the phase shifts ($\delta_L^a$) that were calculated using the Equations (5) and Equation (6) are shown for some values of the $L$ angular momentum, furthermore, the exact theoretical values of the phase shifts ($\delta_L^c$) that have been calculated using the static potential reported in reference [12] are also shown in Table 1, it is observed that the phase shifts ($\delta_L^c$) that were fitted in this way are not in agreement with the exact theoretical values ($\delta_L^c$). This is due that the elastic differential cross section has values very small for some $\theta_i$ values, therefore, it is necessary to introduce quantities ($w_i$) that give equal weight to the $\Delta_i$ quantities in Equation (5), then we take $w_i = (\Delta_i)^{-1}$ and the Equation (5) becomes the Equation (8).

$$\sum_{\theta_i=1}^{N} (w_i\Delta_i)^2. \quad (8)$$
Table 1. Phase shifts and setting parameters.

| $L$ | $\delta_L^a$ | $\delta_L^b$ | $\delta_L^c$ | $\alpha$ |
|-----|---------------|---------------|---------------|----------|
| 0   | 0.3026        | 0.9446        | 0.9463        | 2.0022   |
| 1   | 0.3898        | 0.0857        | 0.0856        | 1.9999   |
| 2   | -0.0933       | 0.0109        | 0.0109        | 2.0001   |
| 3   | -0.0454       | 0.0015        | 0.0015        | 2.0007   |
| 4   | 0.0626        | 0.0003        | 0.0002        | 2.0020   |
| 5   | -0.0032       | $-1.1 \times 10^{-5}$ | $3 \times 10^{-5}$ | -- |
| 6   | -0.0848       | $-3.4 \times 10^{-5}$ | $4 \times 10^{-6}$ | -- |

In Table 1 the values of the phase shifts ($\delta_L^b$) that were fitted using the Equation (8) are also shown, it is observed that when it is used the Equation (8) our results for the phase shifts ($\delta_L^a$) are in a very good agreement with the exact theoretical values ($\delta_L^c$).

To continue implementing the method, we now propose a semi-empirical potential that is shown in Equation (9), note that it is a modification of the exact theoretical static potential that models the collision of electrons with hydrogen atoms (see reference [12]).

$$V(r, \alpha) = -(1 + \frac{1}{r}) \exp(-\alpha r).$$

The values of the $\alpha$ parameter that were obtained using the Equation (7) and the bisection method are shown in Table 1 for different values of the $L$ angular momentum, for these calculations we used the ($\delta_L^a$) values as the $\delta_L$ values in Equation (7). Note that we did not report values for the $\alpha$ parameter for high values of angular momentum ($L = 5, L = 6$) because the phase shifts are too small for these values and therefore have less physical importance in the sum in Equation (1). On the other hand, the mean value of the $\alpha$ parameter is equal to 2.00098 which only differs from the exact theoretical value “2” with an error of 0.049%, the latter means that our method gives very good results; we also test the method using a semi-empirical potential that depends on two parameters and it is shown in Equation (10).

$$V(r, \alpha, \beta) = -(1 + \frac{\beta}{r}) \exp(-\alpha r).$$

The values that we calculated for the potential parameters in Equation (10) were $\alpha = 1.9990$ and $\beta = 0.9972$ which have errors with respect to the theoretical values of $-0.05\%$ and $-0.28\%$ respectively. Our results are very good again.

4. Conclusions

In this theoretical work was developed a simple method which allows to study the inverse problem in scattering theory by means of semi-empirical potentials; with this approach it is possible to calculate the phase shift from the experimental data of the elastic differential cross section and with these last values it is possible to fit the settings parameters of the potentials. The method was tested with great results to the collision process of electrons with hydrogen atoms.

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