A system of first-order differential equations to calculate the Jost functions

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Abstract. Theoretical or experimental studies of the interactions between quantum particles are very important in physical sciences because from them it is possible to know the properties of the systems, therefore, the Jost functions are very important in Quantum Scattering Theory because they allow to carry out unified studies on bound states, scattered states, virtual states and resonance states. In this work a new method to calculate the Jost functions is presented, this method is based on a system of first order differential equations and has the advantage that the solutions of the problem can be calculated by solving the system of differential equations from the origin or from infinity, therefore, it facilitates calculations when systems are modeled with singular potentials at the origin. We tested this method by modeling the collision of an electron with a hydrogen atom in its ground state at low energies (10 eV) and found very good results.

1. Introduction
The Jost function is the theoretical concept which allows to do unified studies on bound states, virtual states, scattered states and resonant states which can be originated in the interactions between two quantum systems. In theory of Quantum Collisions, the Jost function plays a very important role due that it is directly related with the scattering matrix $S$. In the literature there are many articles related with this function.

In 1998 the authors in [1] presented an exact method to calculate the Jost functions and the Jost solutions for not central potentials. In 1999 the authors in [2] used a comparison method to study the scattering by a complex potential, where the Jost function is obtained after finding the regular solution of the problem. Also, in 1999 the authors in [3] proposed a method to calculate the Jost function for a singular and repulsive potential, in which the Schrödinger equation is replaced by a first order differential equations system.

In 2006 the authors in [4] proposed a numeric method to study the inelastic collisions by means of Jost solutions. Moreover, in 2006 the authors in [5] used an integral representation for the Jost function. In 2009 the authors in [6] studied the Volterra integral equations for the regular solution and Jost solution, also in 2009 the authors in [7] developed a systematic and exact procedure to calculate the coefficients of the expansion in series of the Jost function, in 2011 a differential equation was found by the authors in [8] to calculate the Jost Function.

All the above-mentioned methods for computing Jost functions have to solve equations using initial conditions at the origin, which causes great difficulties when systems are modeled using
potentials that have large singularities at the origin (greater than $r^{-2}$). This raises the following question, is it possible to develop a method to compute the Jost functions using initial conditions at infinity? To answer the last question, in this work a method was developed to calculate the Jost functions, it is based on a system of first order differential equations in which it is possible to use initial conditions at the origin or at infinity. Later, this method was applied to study the elastic scattering of electrons by hydrogen atoms and we obtained very good results.

2. Methodology

The scattering process of a particle having wave number $k$ and mass $m$ by a local, spherical and symmetric potential $V(r)$ is fully described when the regular solution $\psi_L(k,r)$ of Schrödinger’s radial equation is known, i.e., when the Equation (1) is solved (see reference [9]).

$$\frac{d^2}{dr^2}\psi_L(k,r) + \left[k^2 - \frac{L(L+1)}{r^2} - U(r)\right]\psi_L(k,r) = 0,$$

where $U(r) = 2mV(r)/\hbar^2$ is the reduced potential, $k^2 = 2mE/\hbar^2$, $L$ is angular momentum and $E$ is the energy of the system. For short-range potentials (decaying faster than $r^{-3}$ at infinity) and potentials that are less singular than $r^{-2}$ at the origin $r = 0$, The regular solution of Equation (1) satisfies the boundary conditions in Equation (2) and Equation (3) (see reference [9]).

$$\psi_L(k,r) \xrightarrow{r \to \infty} i^{2L+1} [F_L(k)h_L^-(kr) - F_L(-k)h_L^+(kr)],$$

$$\psi_L(k,r) \xrightarrow{r \to 0} j_L(kr).$$

In Equation (2), $F_L(k)$ are the Jost functions and $h_L^\pm(kr)$ are the Riccati-Hankel functions, while in Equation (3) $j_L(kr)$ are the Riccati-Bessel functions. The Jost functions are related to the scattering matrix $S$ by means of Equation (4) [9],

$$S_L(k) = \frac{F_L(-k)}{F_L(k)}.$$  

Following Sofianos S A [3, 10] and Alcalá Varilla L A [8], the method to solve Equation (1) involves proposing the expression in Equation (5) like regular solution for all $r$ (see references [3, 8, 10]).

$$\psi_L(k,r) = i^{2L+1} \left[ f_L(k,r)h_L^-(kr) - f_L(-k,r)h_L^+(kr) \right],$$

where $f_L(k,r)$ are known as the Jost solutions and they satisfy the expression given in Equation (6) [8],

$$h_L^-(kr)\frac{d}{dr}f_L(k,r) - h_L^+(kr)\frac{d}{dr}f_L(-k,r) = 0,$$

and when $r$ tends to infinity, the Jost solutions become the Jost functions (see Equation (7)) [8],

$$f_L(k,r) \xrightarrow{r \to \infty} F_L(k).$$

On the other hand, the authors in [8] used the Equation (1), Equation (5), and Equation (6) for showing that the Jost solutions can be calculated solving the Equation (8) [8].
\[ f''_L(k, r) - \left[ \frac{U'(r)}{U(r)} + 2 \frac{h^+_L(kr)}{h^+_L(kr)} \right] f'_L(k, r) - U(r) f_L(k, r) = 0, \tag{8} \]

where the prime index means to derive with respect to \( r \).

The authors in [8] showed that for regular potentials Equation (8) can be solved using any real value for the initial conditions at \( r = 0 \) and it is always found the same values for the Jost functions, but when the potentials are irregular at the origin, it is not possible to solve the Equation (8) in a simple way, the Lenard-Jones potential is an example of an irregular potential at the origin, for this kind of potentials we have to use different shapes to solve the Equation (8).

In this work an alternative method is presented to solve the Equation (8), it involves changing the Equation (8) by a system of first-order differential equations that can be solved from initial conditions at infinity; to carry out the above we propose the expression in Equation (9).

\[ \zeta_L(k, r) = \frac{1}{f_L(k, r)} \frac{d}{dr} f_L(k, r). \tag{9} \]

From Equation (9), it is noted that when \( r \) tends to infinity the new \( \zeta_L(k, r) \) functions tend to zero, i.e., \( \lim_{r \to \infty} \zeta_L(k, r) = 0 \), the above happens because the Jost solutions tend to be constant when \( r \) tends to infinity and thus the derivatives of them become zero for \( r \to \infty \).

If now, the Equation (9) is introduced into Equation (8) it is found the Equation (10) for \( \zeta_L(k, r) \) functions,

\[ \zeta'_L(k, r) + \zeta^2_L(k, r) - \left[ \frac{U'(r)}{U(r)} + 2 \frac{h^+_L(kr)}{h^+_L(kr)} \right] \zeta_L(k, r) - U(r) = 0, \tag{10} \]

and from Equation (9) it is found an integral equation to calculate the Jost functions (see Equation (11)).

\[ F_L(k) = f_L(k, a) \exp\left[ \int_a^\infty \zeta_L(k, t) \, dt \right], \tag{11} \]

where \( a \) is any value of \( r \). Therefore, Equation (10) and Equation (11) can be used to calculate the Jost functions, in that process it is needed to know the value of \( f_L(k, a) \) and the initial condition to solve Equation (10). Thus, using Equation (5) and its first derivative it is possible to find the Equation (12).

\[ f_L(k, r) = \frac{1}{k} [h^+_L(kr) \frac{d}{dr} \psi_L(k, r) - \psi_L(k, r) \frac{d}{dr} h^+_L(kr)], \tag{12} \]

where the Equation (6) was also used. Equation (12) can be used to calculate the value of \( f_L(k, a) \) and the initial condition of Equation (10). Remember that Equation (10) can also be solved using \( \lim_{r \to \infty} \zeta_L(k, r) = 0 \) as an initial condition. On the other hand, when the potentials are regular at origin it is easy to prove that \( f_L(k, a = 0) = 1 \) and \( \zeta_L(k, r = 0) = 1 \). Therefore, for regular potentials Equation (11) becomes the Equation (13).

\[ F_L(k) = \exp\left[ \int_0^\infty \zeta_L(k, t) \, dt \right]. \tag{13} \]

3. Results and discussion

Now, we test the method proposed in this paper to calculate the Jost function, modeling the scattering process of electrons by hydrogen atoms. For that, it is known that the interaction between these particles is mainly due to the potentials in Equation (14) and Equation (15) (see references [11, 12]).
\[ V_{\text{est}}(r) = -(1 + \frac{1}{r}) \exp(-2r), \quad (14) \]
\[ V_{\text{pol}}(r) = -\frac{4.5}{2r^4} [1 - \exp\{- (r/2)^6\}] \cdot (15) \]

In Equation (14) and Equation (15), \( V_{\text{est}} \) and \( V_{\text{pol}} \) are the static potential and the polarization potential respectively, thus the total potential is \( V(r) = V_{\text{est}}(r) + V_{\text{pol}}(r) \). It is observed that this potential is regular at the origin, therefore, Equation (13) can be used to calculate the Jost functions and after that, we can find the phase shifts \( \delta_L \) of the collision from \( F_L(k) = |F_L(k)| \exp(-i\delta_L) \): we modeled the scattering process using a collision energy of 10 eV. Then, Equation (10) was solved and Figure 1 shows the real and imaginary parts of \( \zeta_L(k, r) \) function. It can be seen from Figure 1(a) that the real part of \( \zeta_L(k, r) \) function tends to zero when \( r \) tends to infinity, and from Figure 1(b) it is observed that the imaginary part of \( \zeta_L(k, r) \) function also tends to zero when \( r \) tends to infinity, so we can say that the \( \zeta_L(k, r) \) function has the expected behavior at infinity, i.e, \( \lim_{r \to \infty} \zeta_L(k, r) = 0 \).

On the other hand, Table 1 shows some values of the Jost functions \( F_L(k) \) for various values of angular momentum \( L \), later with the phase of \( F_L(k) \) function we calculated the phase shifts \( \delta_L \) of this work and these are shown in Table 1, the phase shifts \( \delta_L \) that were reported by the authors in [11] are also shown in Table 1. It is observed that our results for the phase shifts \( \delta_L \) are very in agreement with the \( \delta_L \) calculated in [11], this shows in a simple way that our method gives excellent results.

**Figure 1.** Solution of Equation (10) for the elastic collision \( e^- + H(1s) \) at an energy of 10 eV and angular momentum \( L = 0 \); (a) real part and (b) imaginary part

**Table 1.** Phase shifts for the collision \( e^- + H(1s) \).

| \( L \) | \( F_L(k) \) | \( \delta_L^a \) | \( \delta_L^b \) |
|---|---|---|---|
| 0 | 0.17051 – 0.325791i | 1.0886255 | 1.0887879 |
| 1 | 0.46479 – 0.154905i | 0.3216971 | 0.3216620 |
| 2 | 0.60638 – 0.061274i | 0.1007066 | 0.1006706 |
| 3 | 0.70347 – 0.024554i | 0.0348902 | 0.0348725 |
| 5 | 0.80626 – 0.006561i | 0.0081368 | 0.0081298 |
| 15 | 0.92903 – 0.000322i | 0.0003464 | 0.0003485 |
4. Conclusions
In this theoretical work was developed a simple method which allows to calculate the Jost functions. This method has as advantage that the Equation (10) can be solved using initials conditions at the origin or at infinity, therefore, it facilitates calculations when systems are modeled with singular potentials at the origin. On the other hand, it is noteworthy that the results obtained with the present methodology for the collision $e^- + H(1s)$ are in very good agreement with those reported in the literature.

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