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On The Pole Structure of the S-Matrix for a Square Potential-Well

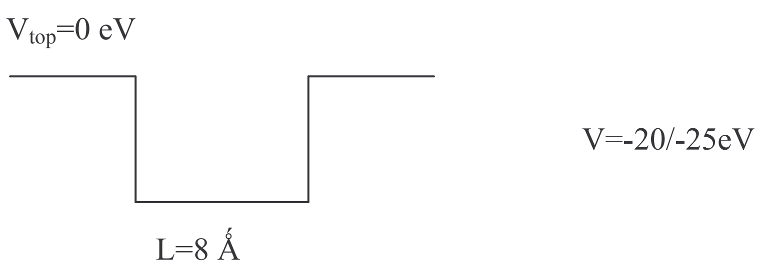
Poles on the scattering matrix or S-matrix exhibit many interesting phenomena that describe the system of interest. These poles either correspond to the bounds states or transmission probability depending on whether the energy of the particle is less then or greater then the asymptotic potential on the left and right. In this short study, the poles of a one-dimensional square well potential are determined and examined. It should be noted that Maple was used to produce the plots and most of the calculations throughout this paper (maple worksheets are attached in the appendix).

S-Matrix

The S-matrix relates the incoming amplitudes (A_L and B_R) for particles approaching a potential with the outgoing amplitudes (A_R and B_L) leaving the potential. Elements for this matrix can be expressed by the transfer matrix elements or T-matrix. It is easily shown that the S-Matrix is

$$S = \begin{bmatrix} \frac{1}{T11} & -\frac{T12}{T11} \\ \frac{T21}{T11} & \frac{det(T)}{T11} \end{bmatrix}$$

The element T_{11} appears in the denominator for each element. Hence, the pole structure on the S-matrix is determined when T_{11}=0. In order to investigate the nature of the poles, a one-dimensional square well is considered. This attractive potential's length is fixed at 8 Å with the depth varied at -20.0 eV and -25 eV.



Remarks on units

As Dr. Gilmore dedicated a whole chapter on units used throughout his book, *Elementary Quantum Mechanics in One Dimension*, it is necessary to say a few remarks about the units used through out this study. It is shown in the picture above that the desired units for energy are electron-Volts (eV) and as a consequence the desired units for length will be angstroms (Å). In order for these units to be properly used, the constants in k (where k is sqrt(2*m*E/ $\hbar^2$)) are as follows; m(mass of electron)=0.911×10^{-27} gm and $\hbar=1.054\times10^{-27}$ erg sec. In addition, for E to be measured in eV the charge, q=1.602×10^{-12} erg, is multiplied in the numerator of the radical and since k is always multiplied by the distance of the potential, L it is only natural to measure length in angstroms (since the product of k is of the order 10^8 cm and one angstrom is 10^{-8}).

Bound states (E<0)

In the case when the energy of the particle is less then asymptotic left and right, E<0, the wavefunctions have the form;

$$\Psi_L = B_L e^{\kappa x}, \text{ with } \kappa = \text{sqrt}(2m(V_L - E)/\hbar^2)$$
$$\Psi_R = A_R e^{-\kappa x}, \text{ with } \kappa = \text{sqrt}(2m(V_R - E)/\hbar^2)$$
$$V_L = V_R = 0$$

with amplitudes, A_L and B_R, set to zero. From these boundary conditions, the transfer matrix elements can now be determined, with T_{11} being of particular interest. The transfer matrix relating the asymptotic left with right is as follows;

$$\begin{bmatrix} A(left) \\ B(left) \end{bmatrix} = \begin{bmatrix} T11 & T12 \\ T21 & T22 \end{bmatrix} \cdot \begin{bmatrix} A(right) \\ B(right) \end{bmatrix}$$

Introducing the boundary conditions, A_L and B_R being equal to zero, and looking at T_{11} the equation is produced;

$$0 = T_{11} * A_R$$

If A_R were equal to zero, then the equation is trivial (all amplitudes inside the square well would be equal to zero, if this were the case). Therefore, to satisfy the boundary conditions T_{11} must be equal to zero and poles or bound states are found.

The element T_{11} is easily found to be

$$cos(k \cdot \delta) + \frac{1}{2} \cdot \left(\frac{\kappa}{k} - \frac{k}{\kappa} \right) \cdot sin(k \cdot \delta)$$

where, $k = \text{sqrt}(2*m*q(E-V)/\hbar^2)$, $\kappa = \text{sqrt}(2*m*q*E/\hbar^2)$, and $\delta = 8$ Å. The poles are calculated graphically with V=-20eV first, then V=-25eV varying E from 0<E<-20 eV and E from 0<E<-25 eV, respectively. When the T_{11} crosses 0, a pole is found, they are shown in the plots below.

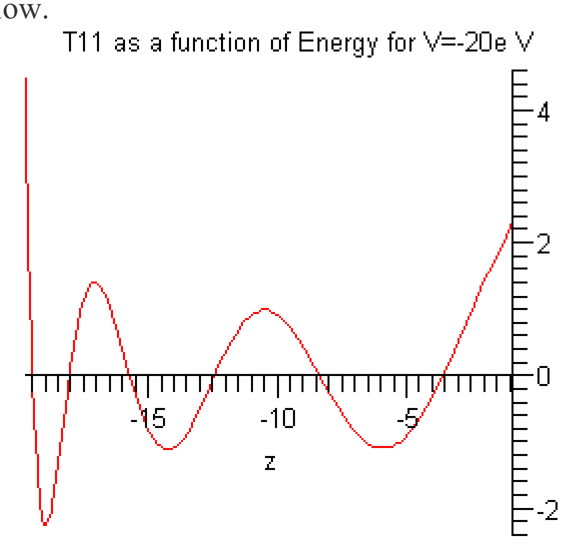


Figure 1-where T_{11} crosses 0; the energy corresponds to a bound state (total of 6)

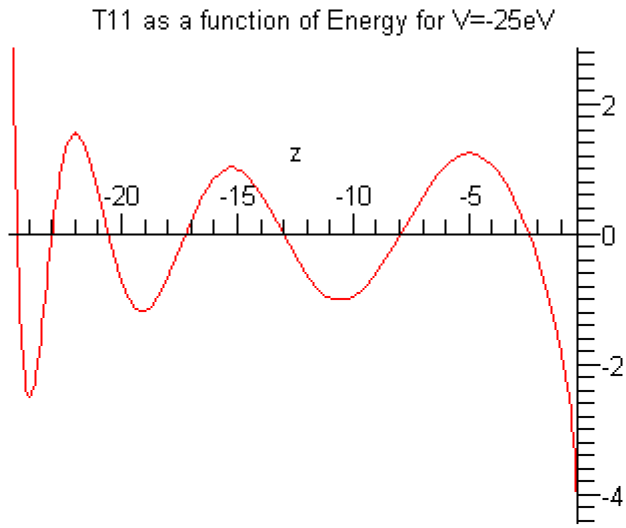


Figure 2-where T_{11} crosses 0; the energy corresponds to a bound state (total of 7)

The bound states for figure 1 (all measured in eV) are −19.52319800, −18.09749157, −15.73849690, −12.47873223, −8.385639050, and −3.634858834 while the bound states for figure 2 are −24.51304076, −23.05567592, −20.63935995, −17.28691048, −13.04157825, −7.994860607, and −2.426037569 (all in eV). It is interesting to note that when the potential was increased another 5 eV, an extra bound state is "formed" at the top of the potential and the energy of the other six are increased ~5eV.

Poles associated with E>0

When the particle is associated with an energy that is greater then 0, scattering occurs. The boundary conditions for scattering are a bit different then the conditions for bound states, therefore T_{11} will be different. If a particle is incident from the left, the asymptotic wave functions will have the following form;

$$\Psi_L = A_L e^{ikx} + B_L e^{-ikx}, \text{ with } k=\text{sqrt}(2m(E-V_L)/\hbar^2)$$
$$\Psi_R = A_R e^{-ikx}, \text{ with } k=\text{sqrt}(2m(E-V_R)/\hbar^2)$$
$$V_L = V_R = 0$$

These are the boundary conditions that shape what T_{11} will look like. It can be shown with quite ease that T_{11} is

$$\cos(kprime\cdot\ \delta) - \frac{i}{2}\left(\frac{kprime}{k} + \frac{k}{kprime}\right)\sin(kprime\cdot\ \delta)$$

where, k'(kprime)=sqrt(2*m*(E-V)/$\hbar^2$), k=sqrt(2*m*E/ $\hbar^2$), and δ=8 Å. There is an obvious difference between the two transfer matrix elements, when E<0 T_{11} was real, while this element is complex. What does this mean?

After some investigation, in order to satisfy the condition that T_{11}=0, the energy has to have a real part and an imaginary part, E is complex. It is a very daunting task to solve this equation with out the aid of a computer (although, I do encourage interested readers to see if they can solve by hand); however when substitutions are made for the cosine and sine term a familiar property is seen. Remember, the sin and cosine term can be represented by the following;

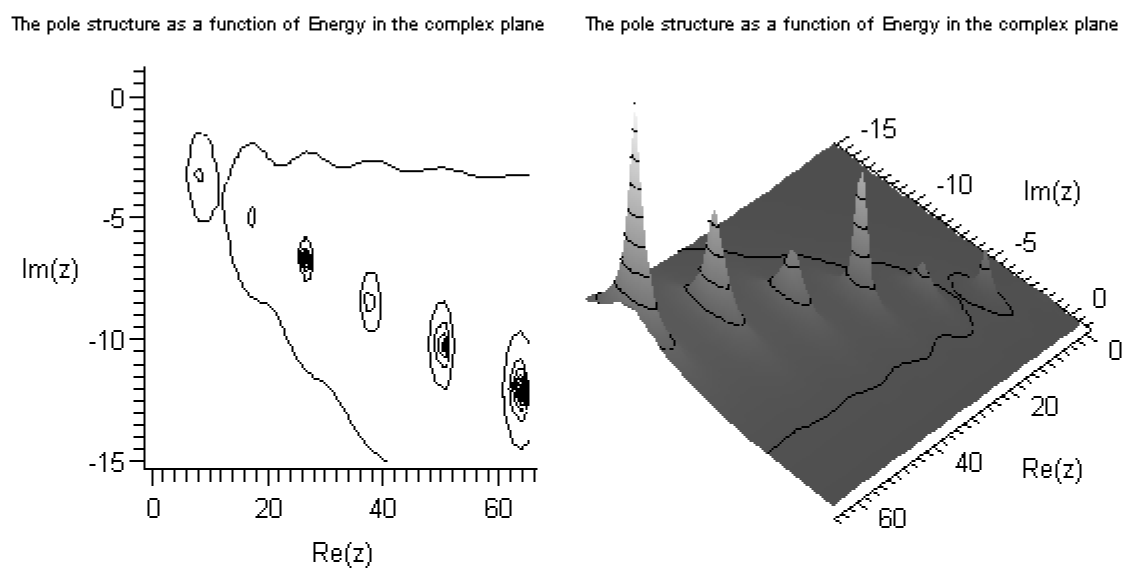
$$cos(k \cdot x) = \frac{e^{i\,kx} + e^{-\,i\,kx}}{2} \qquad sin(k \cdot x) = \frac{e^{i\,kx} - e^{-\,i\,kx}}{2 \cdot i}$$

and leaving the algebra out (can be found in the appendix), the equation can be worked out to;

$$1 = \left(1 - \frac{4 \cdot k' \cdot k}{(k + k')^2}\right) \cdot e^{i \cdot 2 \cdot k' \cdot \delta}$$

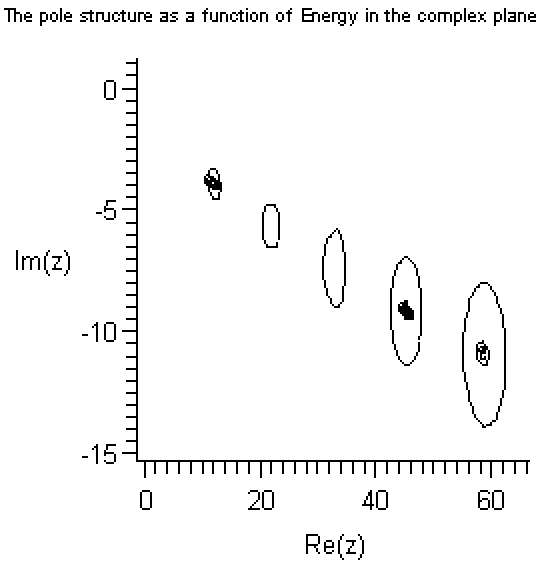
The third term in the equation above $(4k'k/(k+k')^2)$ is the transmission probability in which the potential undergoes only one discontinuous change (encourage readers to work out to see for themselves). Is there is a connection with the transmission probability and complex poles? This is the first indication that a relationship exists between the two and will be explored a bit later.

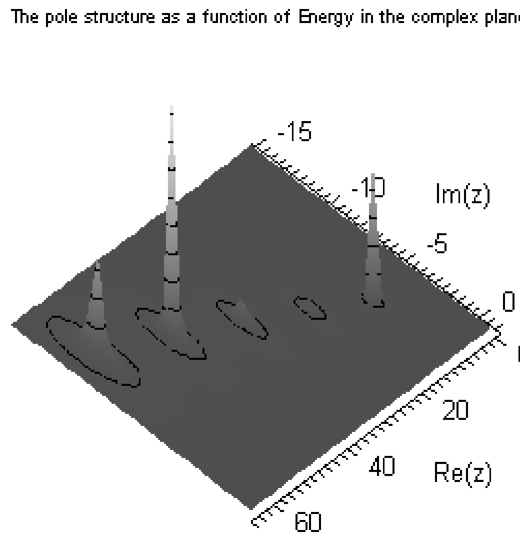
As stated previously, the equation $T_{11}=0$ was solved with the aid of a computer. First, the solutions were obtained using the potential well V=-20 eV, then the well was extended to V=-25 eV. Below are plots of the poles from two different angles, clearly displaying the pole structure in the complex energy plane.



Figures 3(Left) and 4(Right)-Left two dimension view of pole structure (V=-20), Right three dimensional view of pole structure (V=-20). Note that there is a pole near the origin although it is hard to resolve.

Explicitly, the first seven poles are worked out to be E=0.6356243305-0.928664716I, 8.135602450-3.180033221I, 16.81813769-4.934096741I, 26.68201817-6.654186473I, 37.72627705-8.401071367I, 49.95012974-10.19156386I, and 63.35293001-12.03053614I. The next figures show the complex energy plane when the well was extended to V=-25 eV.





Figures 5 and 6-Left two dimension view of pole structure (V=-25), Right three dimensional view of pole structure (V=-25). Note there is a pole that cannot be resolved near 3-1.9I.

Explicitly, the first six poles are worked out to be E=3.230193326-1.903316017I, 11.91963692-3.884782571I, 21.78970431-5.626844608I, 32.83955705-7.346301972I, 45.06850860-9.088876098I, and 58.47598920-10.86926114I. It is interesting that the pole near the origin in figures 4 and 5 has "disappeared" in figures 5 and 6. What happened to this pole, did it really disappear or is it somewhere else on the energy plane?

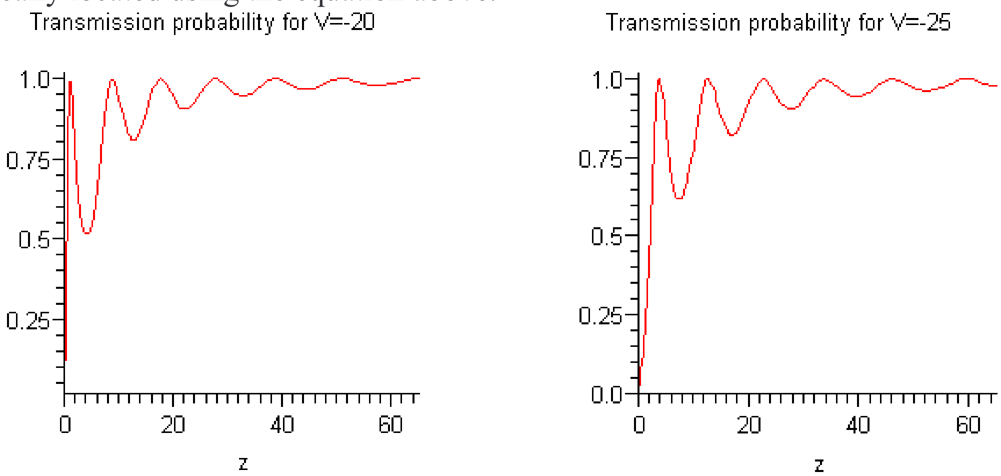
Bound states, Complex Energy Poles, and Transmission Resonances

In this section, all the loose ends that were left unresolved in the previous sections will be tied together. It was shown that the one-dimensional square-well has poles that are real and poles that are complex. Even though these poles, both real and complex, were treated differently (depending on boundary conditions) one might ask, is there a connection between the two? Before this question is approached, the relationship between bound states and transmission resonances peaks will be explored first.

In this paper, transmission resonance has been mentioned with the understanding that the reader is familiar with the term. Briefly, in scattering (in the case considered here, E>0) there exists a probability that the particle incident from the left approaching a potential barrier V will either be transmitted through that barrier or reflected from it. The transmission probability can be expressed as $|1/T_{11}|^2$ and this function can have peaks when result is 1. These peaks or resonances can be found from the following expression;

$$E = \frac{\hbar^2}{2 \cdot m}\left(\frac{n \cdot \pi}{\delta}\right)^2$$

above the potential. Below are the plots of the two potentials considered, with the positive energy being the dependent variable. The peaks are easily seen and can be specifically located using the equation above.



Figures 7(Left) and 8(Right)-Transmission probability for square well potentials V=-20eV and -25eV.

These first seven peaks or resonances for figure 7 are located at the positive energy 1.129664491, 8.75982169, 17.56384873, 27.54174604, 38.69351362, 51.01915151, and 64.51865967. The first six peaks of resonances for figure 8 are located at the positive energy 3.75982169, 12.56384873, 22.54174604, 33.69351362, 46.01915151, and 59.51865967. These energies will be revisited a bit later.

It was previous stated what T_{11} looks like when E>0 and when E<0. What happens when E approaches 0? It is fairly obvious that T_{11} will approach –i*k'sin(k'δ)/2*k for E>0 and –k*sin(kδ)/2*κ for E<0. Both of these functions will blow up as E goes to 0 but if sin(k'δ) is set equal to zero a transmission resonance can occur and similarly if sin(kδ) is set equal to zero a new bound state can occur. This condition describes the transformation of a transmission resonance in becoming a bound state, when sin(k*δ)=0 where k= k=sqrt(2*m*q(-V)/$\hbar^2$). A much more in depth look at this connection between the bound states and transmission resonance is found in *Chapter 25 of Elementary Quantum Mechanics in One Dimension*. Figures 7, 8, 1 and 2 have been combined to illustrate this important connection.

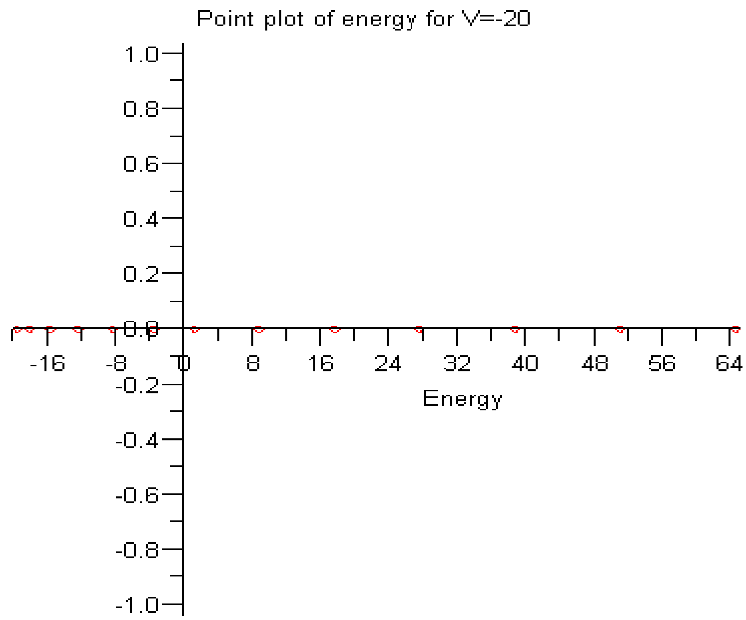


Figure 9-Energy greater then 0 corresponds to a resonance and energy less then zero correspond to a bound state

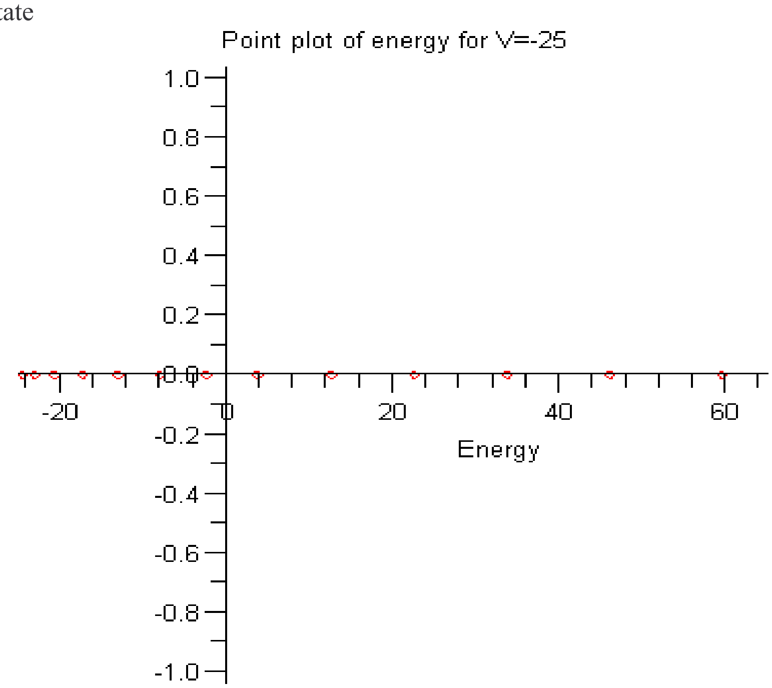


Figure 10-Energy greater then 0 corresponds to a resonance and energy less then zero correspond to a bound state

Before the potential is stretched, there is a resonance at 1.129 eV and 6 bound states. After the potential is increased to -25 eV, the resonances begin at 3.7598 and there is an extra bound state at -2.426 eV. It seems that the resonance at 1.129 eV was transformed into a bound state at -2.426 eV. In fact a more detailed look at the resonances reveal that they have shifted by approximately 5 eV closer to the origin and the bound states are shifted approximately 5 eV away from the origin. A connection has been made between the bound states and the transmission resonance.

After talking a little on the connection between a bound state and a transmission resonance, it is fitting to see what kind of a relationship exits between the bound states and the complex poles that were found. Figures 11 and 12 below are constructed using the complex poles found when E>0 and the bound states, E<0.

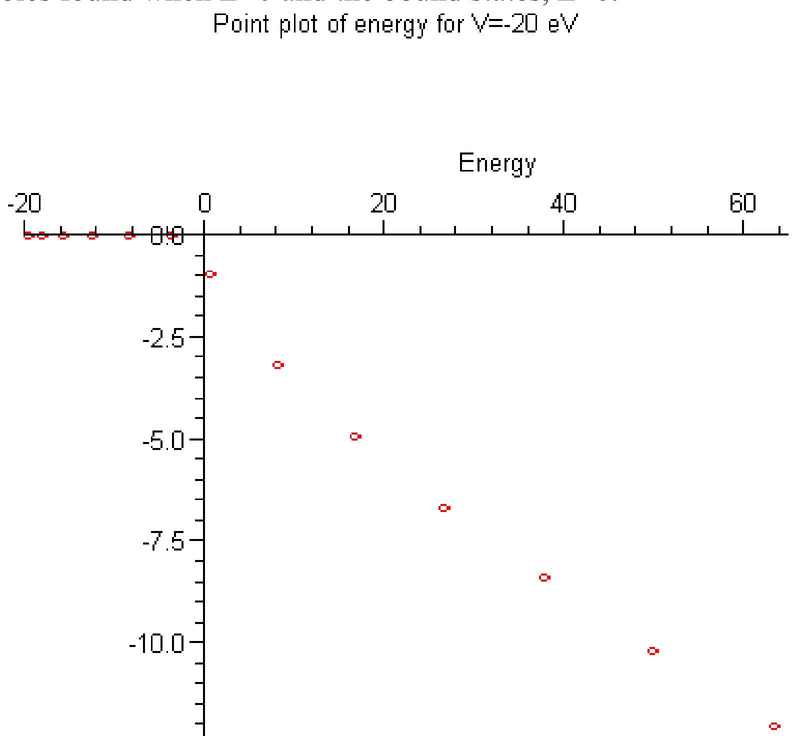


Figure 11- Energy greater then 0 corresponds to a complex pole and energy less then zero correspond to a bound state

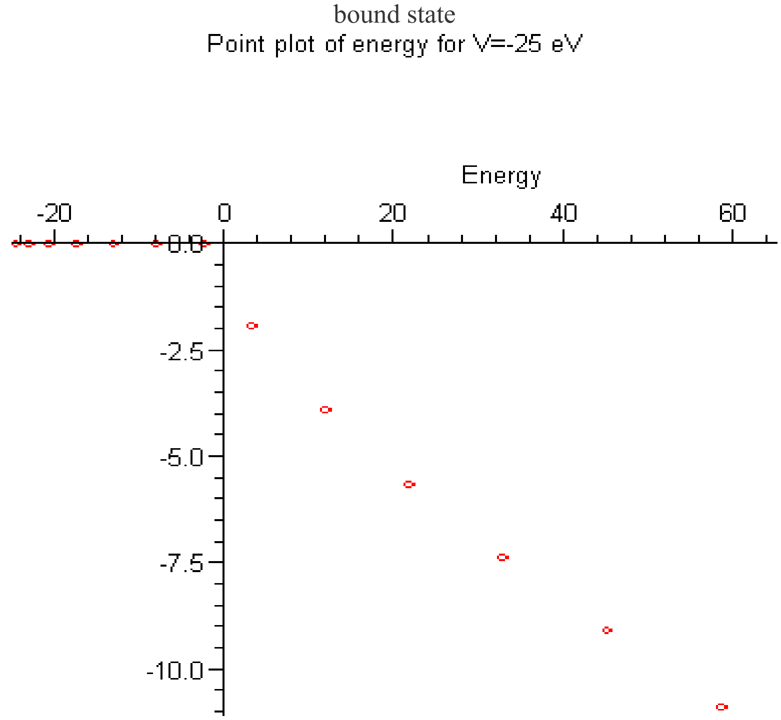


Figure 12- Energy greater then 0 corresponds to a complex pole and energy less then zero correspond to a bound state

It is shown from the two figures, 11 and 12, that the complex poles are shifted from their original position when V=-20 eV to a position closer to the imaginary energy axis. Another interesting artifact about these figures reveal that the pole right next to the imaginary axis, E=0.6356243305-0.928664716I eV, in figure 11 is no longer seen in figure 12 but a new bound state is present. This kind of behavior that exists in these two figures is very similar to that of figures 9 and 10. This is the second piece of information that suggests the complex poles are associated in some way to the transmission probability. Another way that suggests the transmission probability and complex poles are related is to simply take a look at the raw data. The two tables below show only the real energy of the complex poles against the energy of the transmission resonance. It is obvious to see the similarity between the two energies.

Real energy of Complex Pole (eV)	Energy of Transmission Resonance (eV)
0.6356243305	1.129664491
8.135602450	8.75982169
16.81813769	17.56384873
26.68201817	27.54174604
37.72627705	38.69351362
49.95012974	51.01915151

Table 1-Energy of transmission resonance vs. real energy of complex pole for V=-20 eV

Real energy of Complex Pole (eV)	Energy of Transmission Resonance (eV)
3.230193326	3.75982169
11.91963692	12.56384873
21.78970431	22.54174604
32.83955705	33.69351362
45.06850860	46.01915151
58.47598920	59.51865967

Table 2-Energy of transmission resonance vs. real energy of complex pole for V=-25 eV

An explicit relationship between the transmission probability and complex pole structure can now be related. In complex analysis, singularities or poles are normally associated with its residue. When a given function f(z) can be represented by a series of positive and **negative** integer powers of $z-z_o$, the series is said to be a Laurent series. The principal part of this series contains the negative powers and the residue is just the coefficient of the power $1/(z-z_o)$ of this Laurent series.

The complex poles that are associated with $1/T_{11}$ can be classified as simple poles (poles of the first order) and for simple poles the Laurent series is;

$$F(z) = \frac{b1}{z - z0} + a0 + a1(z - z0) + a2(z - z0)^2 + ...$$

remembering that the coefficient b_1 is the residue for that pole. Since $1/T_{11}$ can be expanded in the manner above and complex poles are only contained in the principal part;

$1/T_{11}=r_i/(E-E_{i0})$, where r_i residue of the ith complex pole and E_{i0} is the ith complex pole. Finally the relationship can be made between the complex poles and transmission probability;

$$T(E) = |1/T_{11}|^2 = |r_i|^2/|E-E_{i0}|^2$$

The residues were not calculated for the complex poles in this paper because of time constraints and the ever constant struggle with Maple. The pole structure of the S-matrix for the one dimensional potential well were shown throughout this paper to be intrinsically connected with the bound states and transmission probability.

References

[1] Gilmore, Robert. *Elementary Quantum Mechanics in one Dimension,* Baltimore & London: John Hopkins, 2004.

[2] Gilmore, Robert.