PHYS 6330, Computational Physics III, QM II part

1 Analytic Structure for Spherical Well

In this exercise you will learn about analytic properties of the scattering amplitude. First, have a look at this video – you will produce something similar. The exercise serves to get intuition about scattering/bound state problems and the underlying analytic structure in terms of singularities that manifest themselves as resonances and bound states – and how one transforms into the other as the potential depth changes. For simplicity, you may set $\hbar = m = 1$ in the entire problem. This is also done in the video. Note: here we look at the S-wave only.
Our example is the spherical square well. We want to make an animation that shows the partial-wave amplitude $t_0(k)$ as a function of $k \in \mathbb{C}$. Treating the problem in the complex k-plane is slightly simpler because there is only one Riemann sheet while the complex $E = \hbar^2 k^2/(2m)$-plane has two Riemann sheets.

1. *Bound state problem:* From topic 5, solve the bound-state problem numerically for a well that allows for at least one S-wave bound state. Check the bound state condition to make sure the state exists. Make a plot in which you show the RHS and LHS of Eq. (5.188) for illustration.

2. *The power of analyticity:* Bound state energies are pole positions of t_0 on the positive imaginary k-axis. For the same well as before, search numerically for poles and confirm that their positions (or, position if you have a well with only one bound state) coincide with the bound state energies determined in 1.

3. *Pole trajectories*: Trace the pole movements ("trajectories") in the complex k-plane by plotting $\log |t_0|(k)$ for different $0 < V_0 < V_{\text{max}}$ (make an animation). The logarithm only serves to make poles more visible in the contour plot. This would look like in the video, but you do not have to look for poles for every value of V_0 which is quite cumbersome and takes a lot of time. However, do the animation like in that video, i.e, complex plane to the left and phase shift to the right, to see what effects poles have on the phase shift. Choose the maximal depth of the well, V_{max}, such that there you have at least two bound states.

4. Comment your animation (`Alt+7` to get to commenting mode in Mathematica):

   (a) What do the poles do as the potential gets deeper? Give a qualitative explanation in several complete phrases. In particular, discuss the role of resonances and bound states.

   (b) What happens to the scattering length in the moment the first bound state is at threshold, i.e., at $k = 0$?

   (c) Inform yourself about Levinson's theorem (HZ notes). Comment on how you can confirm that theorem in your animation for the different cases of 0, 1, and 2 bound state(s).

   (d) Have a look at this paper and in particular Fig. 1 and text commenting that figure. Can you see any similarity of the pole trajectories to your animation? Speculate a bit at this point, it is clear that you cannot fully understand the paper.

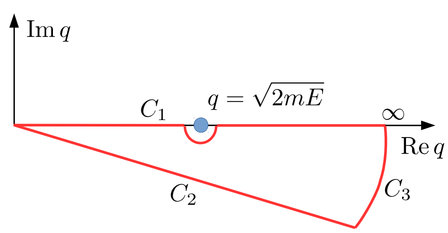
5. Export your animation and make a movie of less than 3MB size of it using, e.g., "handbrake" to reduce file size. Attach that movie to your blackboard submission together with the Mathematica notebook.

2 Lippmann-Schwinger Equation

The goal of this exercise is to numerically solve the Lippmann-Schwinger equation (LSE) in s-wave for the spherical-well potential, see Eq. (7.179). As parameters for the well, use the ones you have employed in a previous computational exercise to calculate the phase shifts as a function of the energy $E = p^2/(2m)$. The solution of the problem is divided into several steps. In your notebook,

- Use sections to follow the same numbering as below.
- Comment all steps in the text environment or inside code with `(* [comment] *)`.
- Comment the logic of your program and which decisions you make, and why.
- Whenever you use a formula from the HZ notes, explicitly refer to it.

First of all, you need to find a solution strategy. In the lecture, we have discussed several alternatives, and you have to choose one suitable for your problem (see discussion below). The numerical procedure is the same for each alternative: Discretize the momenta in the s-wave LSE as discussed to be able to use the matrix inversion trick to solve for $T_0(p', p)$. To your set of “off-shell” points $\{q_i\}$, $i = 1, n$, add an on-shell point $q_{\rm on}$ which increases the dimension of the discretized T_0 and V_0 from n to $n+1$, as discussed. This will provide you the solution for the energy $E = q_{\rm on}^2/(2m)$. For V_0, use the partial-wave projected potential in momentum space calculated in an analytic exercise in the QMII course.
Check the limit considerations in the solution of that exercise. Consider: We found that V_0 falls off sufficienctly rapidly for the integral term in the LSE to converge. A way to solve the LSE, avoiding the singularity in the integration at $q = \sqrt{2mE}$, consists in deforming the original integration from 0 to ∞, called C_1 in the picture below. Indeed, one can integrate along a contour $C_2 = \{q(1 - i\alpha)\}$, $q > 0$ and $\alpha > 0$ of the size of about $\alpha \approx 0.05$ to 0.3. The integral over C_1 equals the integral over C_2, if the integral over the arc segment at large q, called C_3, vanishes. This situation can be illustrated as follows:



The possible problem is: even if the integration along C_1 converges, we have no guarantee that the integration over C_3 vanishes, or that the integration of C_2 converges. This has to be checked, and the test will fail (see exercise below). The reason lies in the sin and cos functions in V_0 that are no longer bound for complex arguments. The way out of this problem is given by several alternatives:

1. Introduce form factors $f(q) = \Lambda^2/(q^2 + \Lambda^2)$ or higher powers thereof to replace $V_0(p', p)$ with $f(p')V_0(p', p)f(p)$ to make the integrand over C_2 convergent and the integral over C_3 vanish. Of course, *after* solving the LSE numerically, you have to take the limit $\Lambda \to \infty$. This is, in fact, a very similar trick we used to calculate Coulomb scattering: We first solved Yukawa scattering and then took the limit $\mu \to 0$ *after* solving the scattering problem.
2. The convergence problem comes from the Fourier transform of the potential, which contains a sharp step. If, instead, you use the Woods-Saxon potential from a previous numerical exercise, and calculate $V_0(p'p)$ from it, you should find a much better and faster converging asymptotic behavior for V_0, especially for complex momenta.

3. You can choose to not deform the integration contour at all. But then your numerics becomes ill defined because your integration hits the singularity at $q = \sqrt{2mE}$. You then have to solve the non-singular W-matrix equation first and follow the steps from the lecture notes to obtain T_0 from there.

Exercise:

1. Check numerically $V_0(p', p)$ at large, real p, p' to confirm the asymptotic behavior found analytically. For this, make a 3D plot in which you show $V_0(p', p)$ multiplied with suitable powers of p, p' to illustrate the behavior.

2. Make now p, p' complex according to the above figure and check whether the integrand of the LSE along C_2 still vanishes sufficiently fast (complex numbers now). This test will fail.

3. Take a decision according to the alternatives outlined above and give reasons for your decision. Have you tried more than one alternative? If so, discuss. Also, discuss with your classmates which strategy could be easier to pursue. You may even decide that each of you tries a different strategy to see what works best.

4. For the numerical solution, you have to first generate your set of off-shell Gauss points, together with weights, $\{(\tilde{q}_i,\, \tilde{w}_i)\}$. This is easily done in Mathematica. However, note that the Gauss points are generated in a given interval, that you can choose, say, $]0, \pi/2[$. Next you have to make a suitable variable transformation (e.g., using tan) to map this finite interval to $]0, \infty[$. This will change the position of the Gauss points and also transform the weights (write a general integral as sum to see this immediately). With your new $\{(q_i,\, w_i)\}$, approximate the integral $\int_0^\infty dx\, \exp(-x)$ and compare to the analytic value to check that your substitution works and you have enough Gauss points (you shouldn't need more than 40 or your program might run slow).

5. Define now the $(n+1) \times (n+1)$ matrices V_0, T_0 and G, the latter containing the q^2 factor and Gauss weights according to Eq. (7.179) and as discussed in class.

6. Solve for T_0 for at least five different energies $E > 0$ and compare it to the analytically known t_0. Make a plot in which you show the analytically known Re $t_0(E)$ and Im $t_0(E)$. In the same plot, show your numerical solutions of the present exercise indicated with large dots. Make a really nice plot this time, please.