Physics 522. Quantum Mechanics II

Problem Set #4 – Scattering

Due Monday, April 16, 2001

Problem 1: Scattering in 1D (From Prof. Finley) (20 Points)
Some of the properties of the 3-dimensional scattering operator, $\hat{S}$, or its matrix elements, $\langle \mathbf{k}' | \hat{S} | \mathbf{k} \rangle$, can be understood by first revisiting the idea in a situation for which we have good intuition, namely the 1-dimensional square barrier.

Consider a 1-dimensional, coordinate-space Hamiltonian of the usual form, with a potential function representing a square barrier,

$$V(x) = \begin{cases} 0, & x < -a \\ V_0 > 0, & -a \le x \le +a \\ 0, & x > +a \end{cases}$$

Looking for energy eigenfunctions, with energy $E < V_0$, we first take them in the (standard) form

$$\Psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx}, & x < -a \\ Ce^{i\kappa x} + De^{-i\kappa x}, & -a \le x \le a, \\ Fe^{ikx} + Ge^{-ikx}, & x > +a \end{cases} \qquad \begin{cases} \hbar k = \sqrt{2mE} \\ \hbar\kappa = \sqrt{2m(V_0 - E)} \end{cases}.$$

As you recall, one may determine the values of the rest of these unknown coefficients in terms of those of any pair, by use of the matching conditions for the wave function and its derivative at the two boundaries. As the potential is symmetric about the origin, the calculation associated with doing this is rather simpler than it might otherwise have been. It is probably better, pedagogically, to re-calculate those coefficients now, but you can go and look them up somewhere if you feel it necessary.

(a) Calculate the elements in the *S*-matrix for this problem, which relates the incoming coefficients to the outgoing ones:

$$\begin{bmatrix} B \\ F \end{bmatrix} = S \begin{bmatrix} A \\ G \end{bmatrix} = \begin{bmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{bmatrix} \begin{bmatrix} A \\ G \end{bmatrix}$$

(b) Please show that the matrix so created is unitary.

(c) Note that, for instance, when there is only a wave incoming from the left, i.e., when G=0, then S_{21} is the ratio of the outgoing, going-toward-the right wave to the incoming, going-toward-the right wave; the absolute square of such a ratio is referred to as the *transmission coefficient*, while its phase is the *phase shift* of the incoming wave. If one begins with only a wave incoming from the right, and defines analogously a transmission amplitude, and, thereby, a transmission coefficient, how are the two so-defined amplitudes related, and their two phases?

(d) Show that the transmission coefficient discussed above is a function of a dimensionless version of the incoming energy, namely $q \equiv E / V_0$, and of course some constants. Please express the transmission coefficient, $T \equiv |S_{21}|^2$ as a function of q and a single, dimensionless constant, α, that can be thought of as a measure of the strength of the interaction relative to the mass of the particle; i.e., determine $T = T(q)$.
The variable q varies from 0 to 1, while the energy and the potential constant, V_0 are appropriate for the form of the wave function given above. What are the values of the transmission coefficient at these limits? Does the graph of this function, as q varies from 0 to 1, have any particular structure, such as maxima or minima?

(e) We could use this same *S*-matrix to discuss various other (related) physics problems. I describe three different ones below.

i. For $E>V_0$, we would maintain k as before, but change the quantity κ to $-ik'$, since, now, k' would be a real quantity: $k' = \sqrt{2m(E-V_0)} < k$. How would this change the function you calculated in part (d)? The range of variation of q is now from +1 to ∞. Is the function $T(q)$ continuous at the point q=1?

ii. If we change the constant V_0 so that it is negative, then it describes a particle of energy E incident on a square well, rather than a square barrier. Making V_0 negative causes q to become negative, so that the description of the scattering process can still be made by our function $T(q)$, except that now q takes on negative values. Take here instead, $q \equiv E / (-V_0)$. If $E>0$, for negative V_0, then the form of the wave function appropriate in part (i), above, with k and k' real, except that now $k' >$ k. \What is now the structure of the graph of T(q) as q varies from 0 to $-\infty$.

iii. If $V_0<E<0$, for negative V_0, then the original form of the wave function now has serious difficulties, since there the wave function must decrease exponentially, only, as it goes off to the far right or the far left. We maintain a reasonable form of the wave function by insisting that we use only real quantities, K, and k', obtained by sending k to iK, with $\hbar K \equiv \sqrt{-2mE}$ and by maintaining the use of k' as in part ii, above. However, in order for our interpretation of the problem to be consistent, we must now arrange NOT to have the terms in the wave function that once were multiplied by B and F. As you recall, only certain values of the energy allow this to occur; the so-called bound-state energy values of the system. How are these bound-state energy values determined? At the bound-state energy values, what is the value of the function $T(q)$?

Problems 2-3 (20 -points)

 (From Cohen-Tannoudji et al)

3. Exercises

a. SCATTERING OF THE p WAVE BY A HARD SPHERE

We wish to study the phase shift $\delta_1(k)$ produced by a hard sphere on the p wave ($l = 1$). In particular, we want to verify that it becomes negligible compared to $\delta_0(k)$ at low energy.

α. Write the radial equation for the function $u_{k,1}(r)$ for $r > r_0$. Show that its general solution is of the form:

$$u_{k,1}(r) = C\left[\frac{\sin kr}{kr} - \cos kr + a\left(\frac{\cos kr}{kr} + \sin kr\right)\right]$$

where C and a are constants.

β. Show that the definition of $\delta_1(k)$ implies that:

$a = \tan \delta_1(k)$

γ. Determine the constant a from the condition imposed on $u_{k,1}(r)$ at $r = r_0$.

δ. Show that, as k approaches zero, $\delta_1(k)$ behaves like* $(kr_0)^3$, which makes it negligible compared to $\delta_0(k)$.

b. "SQUARE SPHERICAL WELL": BOUND STATES AND SCATTERING RESONANCES

Consider a central potential $V(r)$ such that:

$$\begin{aligned} V(r) &= -V_0 \quad &\text{for} \quad r < r_0 \\ &= 0 \quad &\text{for} \quad r > r_0 \end{aligned}$$

where V_0 is a positive constant. Set:

$$k_0 = \sqrt{\frac{2\mu V_0}{\hbar^2}}$$

We shall confine ourselves to the study of the s wave ($l = 0$).

α. *Bound states* ($E < 0$)

(i) Write the radial equation in the two regions $r > r_0$ and $r < r_0$, as well as the condition at the origin. Show that, if one sets:

$$\rho = \sqrt{\frac{-2\mu E}{\hbar^2}}$$

$$K = \sqrt{k_0^2 - \rho^2}$$

* This result is true in general: for any potential of finite range r_0, the phase shift $\delta_l(k)$ behaves like $(kr_0)^{2l+1}$ at low energies.

the function $u_0(r)$ is necessarily of the form:

$$\begin{aligned} u_0(r) &= A\, e^{-\rho r} \qquad &\text{for} \qquad r > r_0 \\ &= B \sin Kr \qquad &\text{for} \qquad r < r_0 \end{aligned}$$

(*ii*) Write the matching conditions at $r = r_0$. Deduce from them that the only possible values for ρ are those which satisfy the equation:

$$\tan K r_0 = -\frac{K}{\rho}$$

(*iii*) Discuss this equation: indicate the number of s bound states as a function of the depth of the well (for fixed r_0) and show, in particular, that there are no bound states if this depth is too small.

β. *Scattering resonances* ($E > 0$)

(*i*) Again write the radial equation, this time setting:

$$k = \sqrt{\frac{2\mu E}{\hbar^2}}$$

$$K' = \sqrt{k_0^2 + k^2}$$

Show that $u_{k,0}(r)$ is of the form:

$$\begin{aligned} u_{k,0}(r) &= A \sin(kr + \delta_0) \qquad &\text{for} \qquad r > r_0 \\ &= B \sin K'r \qquad &\text{for} \qquad r < r_0 \end{aligned}$$

(*ii*) Choose $A = 1$. Show, using the continuity conditions at $r = r_0$, that the constant B and the phase shift δ_0 are given by:

$$B^2 = \frac{k^2}{k^2 + k_0^2 \cos^2 K' r_0}$$

$$\delta_0 = -k r_0 + \alpha(k)$$

with:

$$\tan \alpha(k) = \frac{k}{K'} \tan K' r_0$$

(*iii*) Trace the curve representing B^2 as a function of k. This curve clearly shows resonances, for which B^2 is maximum. What are the values of k associated with these resonances? What is then the value of $\alpha(k)$? Show that, if there exists such a resonance for a small energy ($k r_0 \ll 1$), the corresponding contribution of the s wave to the total cross section is practically maximal.

Problems 4-5 (20 points)

From Sakurai

8. a. Prove

$$\frac{\hbar^2}{2m}\langle \mathbf{x}|\frac{1}{E-H_0+i\varepsilon}|\mathbf{x}'\rangle = -ik\sum_l\sum_m Y_l^m(\hat{\mathbf{r}})Y_l^{m*}(\hat{\mathbf{r}}')\,j_l(kr_<)h_l^{(1)}(kr_>)$$

where $r_<$ ($r_>$) stands for the smaller (larger) of r and r'.

b. For spherically symmetric potentials, the Lippmann-Schwinger equation can be written for *spherical* waves:

$$|Elm(+)\rangle = |Elm\rangle + \frac{1}{E-H_0+i\varepsilon}V|Elm(+)\rangle.$$

Using (a), show that this equation, written in the **x**-representation, leads to an equation for the radial function, $A_l(k;r)$, as follows:

$$A_l(k;r) = j_l(kr) - \frac{2mik}{\hbar^2} \times \int_0^\infty j_l(kr_<)h_l^{(1)}(kr_>)V(r')A_l(k;r')r'^2\,dr'.$$

By taking r very large, also obtain

$$f_l(k) = e^{i\delta_l}\frac{\sin\delta_l}{k} = -\left(\frac{2m}{\hbar^2}\right)\int_0^\infty j_l(kr)A_l(k;r)V(r)r^2\,dr.$$

9. Consider scattering by a repulsive δ-shell potential:

$$\left(\frac{2m}{\hbar^2}\right)V(r) = \gamma\delta(r-R), \quad (\gamma > 0).$$

a. Set up an equation that determines the s-wave phase shift δ_0 as a function of k ($E = \hbar^2k^2/2m$).

b. Assume now that γ is very large,

$$\gamma \gg \frac{1}{R}, k.$$

Show that if $\tan kR$ is *not* close to zero, the s-wave phase shift resembles the hard-sphere result discussed in the text. Show also that for $\tan kR$ close to (but not exactly equal to) zero, resonance behavior is possible; that is, $\cot\delta_0$ goes through zero from the positive side as k increases. Determine approximately the positions of the resonances keeping terms of order $1/\gamma$; compare them with the bound-state energies for a particle confined *inside* a spherical wall of the same radius,

$$V = 0, \quad r < R; \qquad V = \infty, \quad r > R.$$

Also obtain an approximate expression for the resonance width Γ defined by

$$\Gamma = \frac{-2}{[d(\cot\delta_0)/dE]|_{E=E_r}}$$

and notice, in particular, that the resonances become extremely sharp as γ becomes large. (*Note*: For a different, more sophisticated approach to this problem see Gottfried 1966, 131–141, who discusses the analytic properties of the D_l-function defined by $A_l = j_l/D_l$.)

Problem 6: Inelastic Scattering (10 Points)

In many collision problems, above a certain energy the scattering can be inelastic. This generally occurs due to the fact that our approximation of the interaction of two "structureless" particles breaks down when the energy is sufficiently high to excite this other degrees of freedom. For example for a proton incident of an atom with atomic number *Z* we can have:

$p+(Z,A)_{ground} \rightarrow p+(Z,A)_{ground}$ elastic

$p+(Z,A)_{ground} \rightarrow p'+(Z,A)_{excited}$ inelastic: excitation of the atom with proton losing energy

$p+(Z,A)_{ground} \rightarrow n+(Z+1,A)_{ground}$ inelastic: proton scattering into neutral and higher Z atom

If one in interested in the description of the elastic scattering channel, then one can take into account the inelastic channels by introduction an imaginary part to the potential,

$$V(\mathbf{x}) = V_R(\mathbf{x}) - iV_I(\mathbf{x}).$$

The nonHermitian potential is an example of an "open quantum system", in which some of the possible states are external to our description; they constitute a "reservoir".

(a) Starting with the Schrödinger equations for the wave function and its complex conjugate, show that the usual continuity equation for probability and probability current us augmented by a "sink" term:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{J} = -\frac{2}{\hbar}\left(\psi^*(\mathbf{x})V_I(\mathbf{x})\psi(\mathbf{x})\right).$$

(b) With a nonHermitian Hamiltonian, the *S*-matrix is not unitary. Assuming *absorption* is the only inelastic channel, its eigenvalues are then nonunit in magnitude, $|s_l(E)| \equiv \eta_l(E) < 1$.

The absorption cross-section is defined, $\sigma_{abs} = \dfrac{\text{Absorbed flux integrated over all angles}}{\text{Incident flux denisty}}$.

For a spherically symmetric potential, the elastic scattering and absorption cross-sections decompose into partial waves. Show that

$$\sigma_{scat} = \frac{\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)(1-\eta_l)^2,\; \sigma_{scat} = \frac{\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)(1-\eta_l{}^2).$$

(c)Show that the "optical theorem" generalizes to, $\dfrac{4\pi}{k}\mathrm{Im}\left(f(\mathbf{k} \leftarrow \mathbf{k})\right) = \sigma_{total} = \sigma_{scat} + \sigma_{abs}$.