Massachusetts Institute of Technology
Physics Department

Physics 8.322 **Spring 2007**
Quantum Theory II **April 23, 2007**

Assignment 10

Due May 4, 2007, at the end of the day

Announcements

- Please keep an eye on the website, http://web.mit.edu/8.322/, for updates on the problem set.

Reading topics for this period

- Scattering theory: Partial waves, phase shifts, *etc.*
- Formal scattering theory.

Reading Recommendations 10

- Sakurai, Formal development and Born Approximation: §7.1 — 7.3, and Method of Partial Waves: 7.5 — 7.6.
- Gottfried, Partial waves, §8.1; Formal development, 8.2(a); Born approximation, 8.3(a),(b).
- Schiff has a lengthy and pretty good section on scattering theory. §5 for basics and §9 for approximation methods.

Problem Set 10

Topics covered in the problems

- Density of states and Levinson's theorem
- WKB approximation to phase shifts.
- p-wave phase shifts and resonances.
- The K-matrix parameterization
- The phase shift and the radial wave function.

Problems

1. **The density of states and the phase shift**

   Consider a particle interacting with a spherically symmetric potential, $V(r)$ with $V \approx 0$ for $r > b$, but also confined in a very large sphere of radius $R \gg b$.

   (a) Show that the quantization condition on the states with angular momentum ℓ in the sphere is

   $$k_n R + \delta_\ell(k_n) = (n + \ell/2)\pi \tag{1}$$

   where $k^2 = 2mE$.

   (b) Consider two adjacent levels labeled by n and $n+1$. Show that the difference in energy of the two levels, $\Delta E = E_{n+1} - E_n$ is increased or decreased, compared to its value when $V \equiv 0$ (ΔE_0), according to the derivative of the phase shift,

   $$\Delta E - \Delta E_0 = -\frac{k\pi}{mR^2}\frac{d\delta_\ell(k)}{dk}$$

   So an increasing phase shift is a measure of *attraction*, which makes levels more closely spaced.

   This result can be recast without reference to the large sphere's radius as a statement about the density of states.

   (c) Let $d\Delta n_\ell/dk$ be the *change* in the density of states with angular momentum ℓ due to the interaction with the potential. Show that

   $$\frac{d\Delta n_\ell}{dk} = \frac{2\ell+1}{\pi}\frac{d\delta_\ell(k)}{dk}$$

   (d) Show that this is a special case of the general result (presented without proof),

   $$\frac{d\Delta n}{dk} = \frac{1}{2\pi i}\frac{d}{dk}\mathrm{Tr}\ln S(k)$$

   where S is the S-matrix and $n(k)$ is the *total* density of states.

2. **Levinson's Theorem — an example**

   Levinson's theorem theorem states that the difference between the phase shift in the ℓ^{th} partial wave at $k = 0$ and at $k = \infty$ is proportional to the number of bound states with angular momentum ℓ,

   $$\pi N_\ell(\text{bound}) = (2\ell+1)(\delta_\ell(0) - \delta_\ell(\infty))$$

   (a) Use the result of the previous problem to show that Levinson's theorem is equivalent to the statement that the *total number of states* with angular momentum ℓ remains invariant when a potential is introduced.

   The remainder of this problem is dedicated to illustrating this theorem. Consider a finite, attractive potential hole ("a square well") of depth V_0 and range b.

(b) Derive the result quoted in class for the s-wave phase shift,

$$\frac{1}{k}\tan(kb+\delta_0(k)) = \frac{1}{q}\tan qb$$

where $q = \sqrt{k^2+U}$ (and $U = 2mV_0/\hbar^2$).

(c) Show that $\lim_{k\to\infty}\delta_0(k) = 0$. Be careful about ambiguities of $n\pi$.

Now study the phase shift as a function of the depth of the potential, U.

(d) As U increases the potential has more and more bound states. Find the values of U at which new bound states appear.

(e) Study the phase shift as a function of U and k *near* $k = 0$, in order to show that $\delta_0(0)$ jumps by π as the potential increases enough to bind each state. This verifies Levinson's theorem.

3. **WKB approximation phase shifts**

Consider s-wave scattering from a deep, smooth, attractive potential, $V(r) < 0$, with $U(r) = -2mV(r)/\hbar^2$. (Note this definition differs from Problem Set 5, Problem 2.)

(a) Find an expression for the WKB approximation to the phase shift, $\delta_0(k)$. Estimate the number of bound states by applying Levinson's theorem. Does your estimate agree with the sum rule of problem 2 in Problem Set 5?

Now consider Problem 1 of Problem Set 5, which is reproduced in the footnote for your convenience[1]. Note that the potential (shown in Fig. 1) is everywhere positive and has no bound states. In that problem you considered only energies low compared to the height of the barrier. Here you are asked to consider all energies, or momenta $0 \le k < \infty$, but you are only asked to provide qualitative answers.

(b) Explain why the phase shifts computed in this old problem apply to the s-wave in three dimensions.

(c) Explain why $\delta_0(0) = \delta_0(\infty) = 0$ in this problem.

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[1] Consider a particle moving on the half-line $x \ge 0$ in the presence of a potential like the one shown in Figure 1.

Suppose the potential barrier is very "high" compared to the energy. Then, qualitatively, there are two types of solutions, those that live primarily inside the potential and those that live outside.

A little terminology: for "generic" choices of the energy (always low compared to the barrier height) the particle lives outside the barrier and has a small amplitude to tunnel in. For "special" choices of the energy, the particle lives inside the barrier and has a small amplitude to tunnel out. Whatever the energy, we can parameterize the solution to the Schrödinger equation by a "phase shift" at large x:

$$\psi(x) \propto \sin(kx+\delta(k)), \text{ for } x \gg b$$

where b is the "range" of the interaction and $k = \sqrt{2mE/\hbar^2}$. $\delta(k)$ is the shift in the phase of the wave function compared to the case $V(x) = 0$, where $\psi_0(x) \propto \sin kx$.... [Problem continues.]

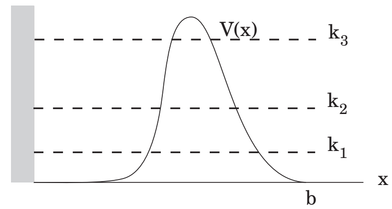

Figure 1: A high potential and a low energy state.

(d) Assume, for example, that the potential is such that there are **three** "special" values of the energy, corresponding to $k_{1,2,3}$ for the potential shown in the figure. Why does the phase shift increase by approximately π between one special value and another? [It will help to remember Problem Set 1, problems 3 and 4.] What is the phase shift for non-special values of k where the WKB approximation applies, both at small k and large k?

(e) Sketch the s-wave phase shift accurately as a function of k.

4. **p-wave phase shift**

The object here is to explicitly find a phase shift in a partial wave with $\ell \neq 0$, and to see the striking phenomena that can occur. Consider an attractive potential hole, $V(r) = -V_0\theta(b-r)$, and as usual, define $U = 2mV_0/\hbar^2$ and $k^2 = 2mE/\hbar^2$.

(a) How large must U be in order for the potential to have one p-wave bound state? Express your result as a condition on the dimensionless quantity $\gamma^2 = Ub^2$. Let γ_0 be the value of γ that gives a bound state at zero binding. You may want to look at Schiff (3rd edition) §15. In any case you'll need to know some spherical Bessel's functions.

(b) In lecture I quoted a general (not just for the potential hole) expression for the phase shift for the ℓ^{th} partial wave in terms of the logarithmic derivative of the radial wave function at a point b outside the range of the potential,

$$\tan\delta_\ell(k) = \frac{xj'_\ell(x) - j_\ell(x)\beta_\ell(k)}{xn'_\ell(x) - n_\ell(x)\beta_\ell(k)}$$

where $x = kb$ and

$$\beta_\ell(k) = \frac{b}{R_\ell(k,r)}\frac{\partial R_\ell(k,r)}{\partial r}$$

and $R_\ell(k,r)$ is the radial wave function (the factor of r has not been explicitly extracted, so in the case of no interaction, $R_\ell(k,r) = j_\ell(kr)$).

Derive this expression.

(c) Find an expression for the p-wave ($\ell = 1$) phase shift, $\delta_1(k)$, for the potential hole. Write your result as a function of the dimensionless variable kb and the parameter γ. Plot the partial wave cross section, $\sigma_1(k) = 12\pi\sin^2\delta_1(k)/k^2$ for $\gamma = \gamma_0/2$, $\gamma = 0.93\gamma_0$, $\gamma = 0.98\gamma_0$,$\gamma = 1.05\gamma_0$ and $\gamma = 1.5\gamma_0$. [Note: You will need to use Matlab, Mathematica (or something equivalent) to make these plots. You may find the properties of spherical Bessel functions enumerated in Abramowicz and Stegun useful. Note, also, that it is quite a bit simpler to get these programs to plot $\sin^2\delta$ than to plot δ itself.]

5. **The K-matrix**

It is often difficult to parameterize the S-matrix in a way that is consistent with unitarity. For example, as described in lecture, a pole just below the real axis (in k^2) in S shows up as a resonance. An adequate parametrization of a resonance is, therefore,

$$S_1(k) = \frac{k^2 - k_1^2 - ik\gamma_1}{k^2 - k_1^2 + ik\gamma_1}$$

with $\gamma_1 \ll k_1$.

(a) Show $S_1(k)$ is unitary for real k^2. Where are the poles in $S_1(k)$ in the complex k-plane? In the complex k^2-plane? Which pole is near the physical region for scattering? Does $S_1(k)$ have a cut (as a function of k^2)? Is this analytic structure consistent with the general restrictions on S?

(b) Suppose S has two nearby resonances. Show that you *cannot* parameterize this behavior by adding the S-matrices corresponding to two independent resonances, *ie.* show that

$$S_k = \frac{k^2 - k_1^2 - ik\gamma_1}{k^2 - k_1^2 + ik\gamma_1} + \frac{k^2 - k_2^2 - ik\gamma_2}{k^2 - k_2^2 + ik\gamma_2}$$

is not in general unitary.

The K-matrix formalism solves this problem — and others too. Consider s-wave scattering in three dimensions (for simplicity). The radial wave function, $u(r)$, must vanish at the origin. The S-matrix is defined by $\lim_{r\to\infty} u(r) = e^{-ikr} - S(k)e^{ikr}$. The K-matrix is defined by a different parametrization:

$$\lim_{r\to\infty} u(r) \propto \sin kr + kK(k)\cos kr \qquad (2)$$

K is a real function of (real) k^2 because unlike S, the boundary condition that determines $K(k)$ is real for real k and invariant under $k \to -k$ (up to an overall sign).

(c) Solve for $S(k)$ as a function of $K(k)$. Show that $S(k)$ *is unitary for any real function* $K(k)$ and that it has the expected square root branch cut as a function of k^2.

(d) Propose a parametrization of $K(k)$ that will generate an S-matrix with two nearby resonances. Make sure the resonances are in the proper location in the complex k-plane. Note that the resulting S-matrix is *always* unitary. [You do not have to do any algebra!]

(e) Parameterize very low energy scattering by making a Taylor expansion of $K(k)$,

$$K(k) = c_1 + c_2 k^2 + \ldots$$

find the condition on c_1 such that there is a very weakly bound state or a very nearly bound virtual state. Return to the definition of $K(k)$ in eq. 2, and show that with this condition on c_1, there is indeed a bound or virtual state at the appropriate (imaginary) momentum. [$-c_1$ is usually called the "scattering length" for reasons that will become clear soon.] Note that these poles in the S-matrix have a different origin than the poles you created in part (d).

6. **A formula for the phase shift**

Problem shifted to next problem set.