Massachusetts Institute of Technology
Physics Department

Physics 8.322 **Spring 2007**
Quantum Theory II **May 7, 2007**

Assignment 11

DUE MAY 16, 2007, AT THE END OF THE DAY

Announcements

- Note the due date. This is the last problem set, and it's due on the last day allowed by the faculty rules.
- I've put some problems on this problem set that we may not get to. If you start to work on this, begin with the first two problems. Some time next week I will confirm how many of the remaining problems will be required.

Reading topics for this period

- Formal scattering theory; Born Approximation; Separable Potential

Reading Recommendations 12

- Separable potentials: Gottfried and Yan, §8.2(b). Separable potentials are discussed in pursuit of a research problem in R. Jaffe and L. Williamson, Annals Phys. **282** 432-448 (2000), hep-th/9907199.
- The original references to Feshbach resonances are: H. Feshbach, Ann. Phys. (NY), **5**, 357 (1958); U. Fano, Nuovo Cimento **12**, 154 (1937) and Phys. Rev. **124**, 1866 (1961). You can also read about them in R. Jaffe and A. Jain, Phys. Rev. **D 71**, 034012 (2005),hep-ph/0408046.

Problem Set 12

Topics covered in the problems

- Scattering on a strip and the Landauer conductivity.
- Analyzing a scattering amplitude.
- Scattering of thermal neutrons — Wigner's R-matrix method.
- Spin dependent scattering in the Born Approximation.

Problems

1. **Scattering on a strip and the Landauer conductivity**

   Electrons on the surface of a semiconductor can be constrained to move in a strip. Such a system is shown in the Fig. (1). For simplicity we take the width of the strip

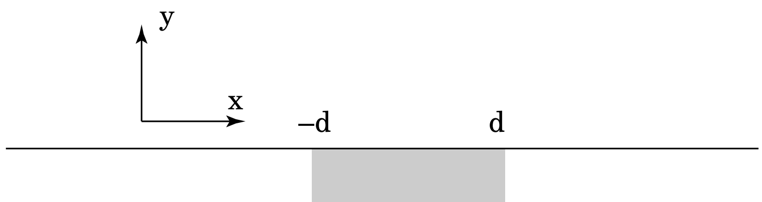

Figure 1: A strip of unit width with a region of interaction bewteen $x = -d$ and $x = d$.

   to be 1 and set $2m = 1$. The confining forces require that the electron wavefunction vanishes at $y = 0$ and $y = 1$. In the region between $x = -d$ and $x = d$ the electron experiences a potential, $V(x, y)$, with $V = 0$ for $|x| \geq d$. So the Schrödinger equation is

$$-\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)\psi(x, y) + V(x, y)\psi(x, y) = k^2\psi(x, y) \tag{1}$$

   where $k^2 = 2mE$ is the electron energy.

   The object of this problem is to study the reflection and transmission of electrons incident from the left on this region of interaction. This could be studied as a problem in two dimensional quantum mechanics. However it is simpler and much more illuminating to write the y-dependence of the electron wavefunction as a sum over a complete set of states. Let

$$\psi(x, y) = \sum_{n=1}^{\infty} \sqrt{2}\psi_n(k, x)\sin n\pi y$$

   (a) Show that the Schrödinger equation, eq. (1), is equivalent to an infinite set of coupled one dimensional Schrödinger equations,

$$-\psi_n''(k, x) + \sum_{m=1}^{\infty} V_{nm}(x)\psi_m(k, x) = (k^2 - n^2\pi^2)\psi_n(k, x) \tag{2}$$

   Find an explicit expression for $V_{nm}(x)$.

   Thus the state of the system can be thought of as a column vector,

$$|\Psi(k)\rangle = \begin{pmatrix} |\psi_1(k)\rangle \\ |\psi_2(k)\rangle \\ |\psi_3(k)\rangle \\ \cdots \end{pmatrix}$$

with $\langle x|\psi_n(k)\rangle = \psi_n(k,x)$. The components of this vector are called "channels", and the scattering process takes an incident wave in one channel and scatters it into reflected and transmitted waves in the other channels.

As $|x| \to \infty$, only the functions $\psi_n(k,x)$ for which $n\pi < k$ can appear in $\Psi(k,x) = \langle x|\Psi(k)\rangle$. These are called **open channels**. The others must die away exponentially and are called **closed channels**.

Let $|\Phi_n(\pm k)\rangle$ be the solution to the non-interacting case ($V_{nm}(x) = 0$) with a right (left) moving plane wave in the n^{th} channel,

$$\langle x|\Phi_n(\pm k)\rangle \equiv \Phi_n(\pm k, x) = \begin{pmatrix} 0 \\ 0 \\ \cdots \\ \\ \frac{1}{\sqrt{k_n}} e^{\pm i k_n x} \\ \cdots \end{pmatrix}$$

Note the factor of $1/\sqrt{k_n}$ in the normalization, and note also that the "channel momentum", k_n appears in the exponential.

Now let $|\Psi_n^{(+)}(k)\rangle$ be the solution to the full interacting Schrödinger equation that obeys scattering boundary conditions with a left incident wave in the n^{th} channel. The effect of the interaction is to produce components in $\Psi_n^{(+)}$ in all the channels,

$$\langle x|\Psi_n^{(+)}(k)\rangle \equiv \Psi_n^{(+)}(k,x) = \begin{pmatrix} \psi_{1n}^{(+)}(k,x) \\ \psi_{2n}^{(+)}(k,x) \\ \cdots \\ \psi_{mn}^{(+)}(k,x) \\ \cdots \end{pmatrix}$$

You should make sure you understand why the components of $\Psi_n^{(+)}(k,x)$ carry *two* channel indices: one labels the channel in which the particle was incident, the other labels the channel in which the amplitude is observed. The scattering state, $|\Psi_n^{(+)}(k)\rangle$ is defined by standard scattering boundary conditions:

$$\begin{aligned} \lim_{x\to-\infty} \Psi_n^{(+)}(k,x) &= \Phi_n(k,x) - \sum_m^{m_{\max}(k)} R_{mn}(k)\Phi_m(-k,x) \\ \lim_{x\to\infty} \Psi_n^{(+)}(k,x) &= \sum_m^{m_{\max}(k)} T_{mn}(k)\Phi_m(k,x) \end{aligned} \tag{3}$$

where $\mathbf{R}$ and $\mathbf{T}$ are the reflection and transmission *matrices* in this multichannel problem.

(b) What determines the *dimension* $m_{\max}$ of the matrices $\mathbf{R}$ and $\mathbf{T}$?

(c) Show that

$$\sum_m \left(|T_{mn}|^2 + |R_{mn}|^2\right) = 1$$

for each n. Note the role of the factor of $1/\sqrt{k_n}$ introduced into the definition of the components of $\Phi_n(\pm k, x)$.

(d) Write the Lippmann Schwinger equation(s) for this problem.

(e) The free Greens function,

$$\langle n, x|\frac{1}{k^2 - H_0 + i\epsilon}|m, x'\rangle = \delta_{nm} G_n(k, x, x')$$

is the solution to the Schrödinger equation with a point source,

$$\frac{d^2}{dx^2} G_n(k, x, x') + (k^2 - n^2\pi^2) G_n(k, x, x') = \delta(x - x')$$

Find $G_n(x, x', k)$.

(f) Find expressions for the reflection and transmission matrix elements in terms of $\psi^{(+)}_{mn}(k, x)$ and the potential.

Answer:

$$\begin{aligned} T_{mn}(k) &= \delta_{mn} + \sum_{l}^{l_{\max}(k)} \frac{1}{2i} \int_{-d}^{d} dx \frac{e^{-ik_m x}}{\sqrt{k_m}} V_{ml}(x) \psi^{(+)}_{ln}(k, x) \\ R_{mn}(k) &= -\sum_{l}^{l_{\max}(k)} \frac{i}{2k} \int_{-d}^{d} dx \frac{e^{ik_m x}}{\sqrt{k_m}} V_{ml}(x) \psi^{(+)}_{ln}(k, x) \end{aligned} \tag{4}$$

(g) What is the first Born approximation to T_{mn}? to R_{mn}?

In the 1950s Rolf Landauer, a condensed matter physicist working at IBM, analysed the current that could be transmitted through a two dimensional channel like the one you have just studied. In his setup distant ends of the strip are connected by leads to reservoirs of electrons with a fermi momentum k_F. When a voltage is applied across the device a current of electrons flows from one reservoir to the other. See the sketch in Fig. (1).

At very low temperature and with very few impurities or dislocations in the semiconductor, there is nothing to impede the flow of electrons except their transmission through the strip. It is relatively easy to show that there is a linear relation between the impressed voltage and the resulting current. The proportionality coefficient is known as the quantum conductance, σ. Landauer showed that σ has a very simple and elegant form,

$$\sigma(k_F) = \frac{2e^2}{h} \mathrm{Tr}[\mathbf{T}^\dagger(k_F)\mathbf{T}(k_F)]$$

where "Tr" denotes the trace, and $\mathbf{T}$ is the transmission matrix ($[\mathbf{T}]_{mn} = T_{mn}$).

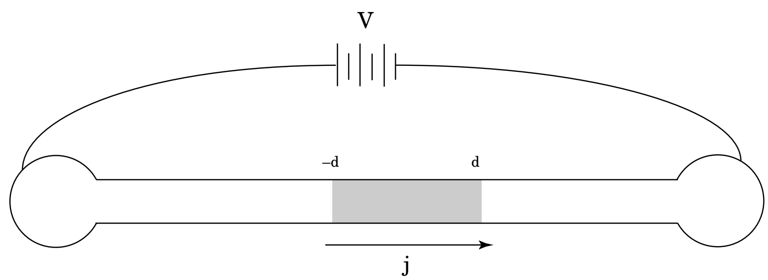

Figure 2: The small strip has been connected to electron reservoirs at either end, both with a fermi momentum of k_F. A current flows through the strip in response to an impressed voltage.

(h) Consider the particularly simple case where there is *no interaction* (!), $V_{nm}(x) = 0$. Plot σ as a function of k_F.

2. **Analyzing a scattering amplitude**

Suppose the elastic scattering amplitude for a certain reaction is given by

$$f(k,\theta) = \frac{1}{k}\left(\frac{g(k)}{k_0 - k - i\Gamma} + Ae^{2i\beta h(k)}\sin(2\beta h(k))\cos\theta\right) \tag{5}$$

where Γ and k_0 are constants characteristic of the potential that produces the scattering. The functions $g(k)$, $h(k)$ and the constant A are not yet determined. Of course $k = \sqrt{2mE/\hbar^2}$ is the deBroglie wavenumber.

(a) What partial waves are active (*i.e.* what values of ℓ)?

(b) What is the function $g(k)$? What is the constant A? How does the function, $h(k)$ behave at small k?

(c) What are the phase shifts in the active partial waves?

(d) What is the differential cross section, $d\sigma/d\Omega$ for general values of k?

(e) What are the partial wave cross sections, σ_ℓ?

(f) Assume $\Gamma \ll 1$. Give an approximation to the total cross section $\sigma(k)$ for $k \approx k_0$.

(g) What is the total cross section for general values of k? What is the imaginary part of the forward scattering amplitude? Do they satisfy the optical theorem?

3. **Scattering of thermal neutrons – Wigners $\mathcal{R}$ Matrix Method**

Neutrons emitted in nuclear fission are slowed by moderators until their energies are "thermal", ie. their typical kinetic energies are of order kT. At room temperature, $kT \approx \frac{1}{40}$ eV.

(a) Find the deBroglie wavelength of a neutron (mass $\approx 10^9$ eV) with kinetic energy $\approx \frac{1}{40}$ eV.

The de Broglie wavelength of a thermal neutron is so large compared to the size of a nucleus ($R_N \approx 10^{-13}$ cm.) that the nucleus looks almost like a point potential to the neutron. However the nucleus exerts a very strong attractive force on the neutron, so strong in fact, that the neutron wavefunction oscillates many times inside the nucleus. When the neutron wavefunction emerges from the nucleus we can parameterize it by the ratio,

$$\mathcal{R} = \psi/\psi'\big|_{R_N}$$

In the absence of interaction, $R_N = 0$ and ψ would vanish at the origin, so $\mathcal{R} = 0$ in the absence of interactions. To calculate $\mathcal{R}$ you would need to know what is going on inside the nucleus. You would start with $\psi(0) = 0$ at the center of the nucleus and then integrate the Schrödinger equation outward until you reached the surface and then you could compute $\mathcal{R}$. Nuclear dynamics are characterized by energy scales of at least tens of KeV. Since $\mathcal{R}$ depends on nuclear dynamics, it doesn't change much as we change $\hbar k$ over thermal (*eg.* room temperature) energy scales. So for thermal neutrons we can take $\mathcal{R} \approx$ constant. The assumption $\mathcal{R} =$ constant is only valid for neutrons whose energies are low compared to the natural excitation energies of nuclei (tens of KeV).

Wigner realized that the scattering of thermal neutrons can be described entirely in terms of the parameter $\mathcal{R}$, which he called the "$\mathcal{R}$-matrix".[1]

(b) Why, for thermal neutrons, is only $\ell = 0$ important for this problem?

The Schrödinger equation for the radial wavefunction with $\ell = 0$ reduces to

$$H\ u(k,r) = -u''(k,r) + \frac{2mV(r)}{\hbar^2}u(k,r) = k^2 u(k,r) \tag{6}$$

Following Wigner we assume the interaction is so short range that $V(r) = 0$ for all $r > 0$, but that the short range interaction with the nucleus affects the wavefunction "at the origin", making $\frac{u}{u'}|_{r=0} = \mathcal{R}$, and we take $\mathcal{R}$ to be a constant (independent of the neutron energy). (This is actually a special case of the $\mathcal{R}$-matrix method applicable when the energy is so low that $kR_N \ll 1$ and the nuclear radius can be ignored entirely.] The object of this problem is to calculate the scattering amplitude and cross section in terms of $\mathcal{R}$.

First, we have to show that $\frac{u}{u'}|_{r=0} = \mathcal{R}$ is an acceptible boundary condition for a quantum problem.

(c) Show that H is a Hermitian operator on the space of square integrable functions that obey the boundary condition $\frac{u}{u'}|_{r=0} = \mathcal{R}$ provided $\mathcal{R}$ satisfies a simple condition. What is it?

[1] Of course $\mathcal{R}$ becomes a matrix if we consider the other labels a neutron can have, like spin. In that case we would have to consider processes where the neutron comes in with spin $\uparrow$ and goes out with spin $\downarrow$. Ignore spin in this problem; it is discussed in the problem on spin orbit interactions later in this problem set.

The s-wave scattering amplitude is entirely characterized by the phase shift, $\delta_0(k)$.

$$u(k,r) \propto e^{-ikr} - e^{2i\delta_0(k)}e^{ikr}, \quad \text{for} \quad r > 0 \tag{7}$$

As usual, we interpret this solution as the superposition of an incoming wave, e^{-ikr}, and an outgoing, "scattered" wave, $e^{2i\delta(k)}e^{ikr}$. When $\mathcal{R} = 0$, $\delta_0(k) = 0$.

Now let's turn to the general case.

(d) Assume $\frac{u}{u'}|_0 = \mathcal{R}$ and solve for the phase shift $\delta(k, \mathcal{R})$, in terms of $\mathcal{R}$.

(e) The S-matrix you found in the previous part has a pole at an imaginary value of $k \equiv i\kappa$. Show that $\lim_{k\to i\kappa}(k - i\kappa)u(k,r) \equiv \phi(\kappa, r)$ is a normalizable solution to the Schrödinger equation if $\kappa > 0$. Explain why this corresponds to a bound state of the neutron, bound to the tiny nucleus. What is its energy? What is the condition on the energy (and on $\mathcal{R}$) for this to be a reliable prediction of Wigners $\mathcal{R}$ matrix theory?

(f) Calculate the total cross section for scattering $\sigma(k, \mathcal{R})$. What happens to the cross section when the bound state you found in the previous part approaches threshold (*ie.* its binding energy goes to zero)?

4. **Spin dependent scattering**

In Problem Set 10 you set up the formalism for spin dependent scattering. In particular you found the expression for the scattering amplitude in the first Born approximation:

$$f_{s,s'}(\vec{k}, \vec{k}') = -\frac{2m}{4\pi}\langle \vec{k}', s'|V|\vec{k}, s\rangle$$

In this problem the object is to study the behavior of spin in a potential with spin-orbit coupling.

Consider a particle with spin-$\frac{1}{2}$, that interacts with a potential of the form[2]

$$V(\vec{x}, \vec{s}) = V(r) + \frac{1}{2m^2c^2}\frac{1}{r}\frac{dV}{dr}\vec{L}\cdot\vec{s}$$

where, of course, $r = |\vec{x}|$.

(a) Compute the scattering amplitude *in the first Born Approximation* and show that it has the form,

$$f_{s,s'}(\vec{k}, \vec{k}') = -\frac{2m}{4\pi}\left(\tilde{V}(q^2) + \tilde{V}_{\text{SO}}(q^2)\; \vec{k}\times\vec{k}'\cdot\vec{S}\right)$$

where $\vec{S} \equiv \langle s'|\vec{s}|s\rangle$, $q^2 \equiv |\vec{k}' - \vec{k}|^2$, and *find the functions* $\tilde{V}$ *and* $\tilde{V}_{\text{SO}}$ *in terms of* $V(r)$.

[2] This is the form we found for the spin-orbit interaction in an electrostatic potential during our study of the hydrogen atom last term. The factor of $\frac{1}{2}$ is from "Thomas precession".

(b) The *spin averaged* differential cross section is given by,

$$\langle\frac{d\sigma}{d\Omega}\rangle = \langle\left|f_{s,s'}(\vec{k},\vec{k}')\right|^2\rangle_{s,s'}$$

where $\langle ... \rangle_{s,s'}$ denotes the *average* over the initial spin and *sum* over the final spin of the spin-dependent cross section. Find $\langle\frac{d\sigma}{d\Omega}\rangle$.

(c) Suppose the initial particle is *unpolarized*. This interaction is capable of producing a polarized scattered particle in the final state. Compute the expected value of the polarization of the final beam as a function of $\vec{k}$, $\vec{k}'$, and the functions $\tilde{V}$, $\tilde{V}_{\text{SO}}$, *etc.* [You will have to read Gottfried and Yan §8.5(b) and (c) in order to answer this question.]