

PHYS 215C In-Class Notes

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1 Scattering

1.1 Suggested References

- Sakurai Ch. 6
- Shankar Ch. 19
- Merzbacher Ch. 11

1.2 Basic Setup

The basic idea in scattering theory is a particle being scattered into a target (particle into target). Other models model two particles moving towards each other and scattering off each other (particle into particle).

1.2.1 Applications

Particle into particle scattering is very prevalent in high energy physics studies (particle accelerators), with traditional subatomic particles like electrons, neutrons, and protons.

Target scattering is used to model particle-particle interactions (particle physics), atoms and ions (atomic/nuclear physics), and interactions within a solid or liquid (condensed matter physics).

1.3 Scattering Approach to e^- Transport in solids

1.3.1 Setup

In this theory we talk about the conduction of electrons in a metal or doped semiconductor. The canonical experiment is a battery providing a potential difference across the material of interest. The conductance, $G = I/V = 1/R$, is what is of interest. There are impurities in the metal or semiconductor that cause scattering of the electrons that are moving under the influence of the potential difference.

1.3.2 Rolf Landauer's Theory (Landauer Transport Theory)

Toy Model Consider a one-dimensional scattering potential that is a finite potential barrier between $x = a$ and $x = -a$ with incident electrons coming from the left with average energy E . (This is actually very relevant in a gated two-dimensional electron gas, where the low energies only allow one mode on the surface dimension.) The theory of this problem is well understood in terms of transmission and reflection coefficients (see the appendix in Sakurai). We will look at the *steady state* system.

First divide the region up into three regions. Region I is $-\infty < x < -a$, region II is $-a < x < a$, and region III is $a < x < \infty$. This gives rise to three wave functions of interest.

$$\begin{aligned}\psi_{\text{I}} &= A_{\text{in}}e^{ikx} + A_{\text{out}}e^{-ikx} \\ \psi_{\text{II}} &= C_1e^{ik'x} + C_2e^{-ik'x} \\ \psi_{\text{III}} &= B_{\text{out}}e^{ikx} + B_{\text{in}}e^{-ikx}\end{aligned}$$

where

$$k = \frac{1}{\hbar}\sqrt{2mE} \quad k' = \frac{1}{\hbar}\sqrt{2m(E - V)}$$

Normally we would solve for these wave functions by matching ψ and ψ' at the boundaries to relate A, B , and C . We can represent the solution via a transfer matrix:

$$\begin{pmatrix} B_{\text{out}} \\ B_{\text{in}} \end{pmatrix} = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} \begin{pmatrix} A_{\text{in}} \\ A_{\text{out}} \end{pmatrix}$$

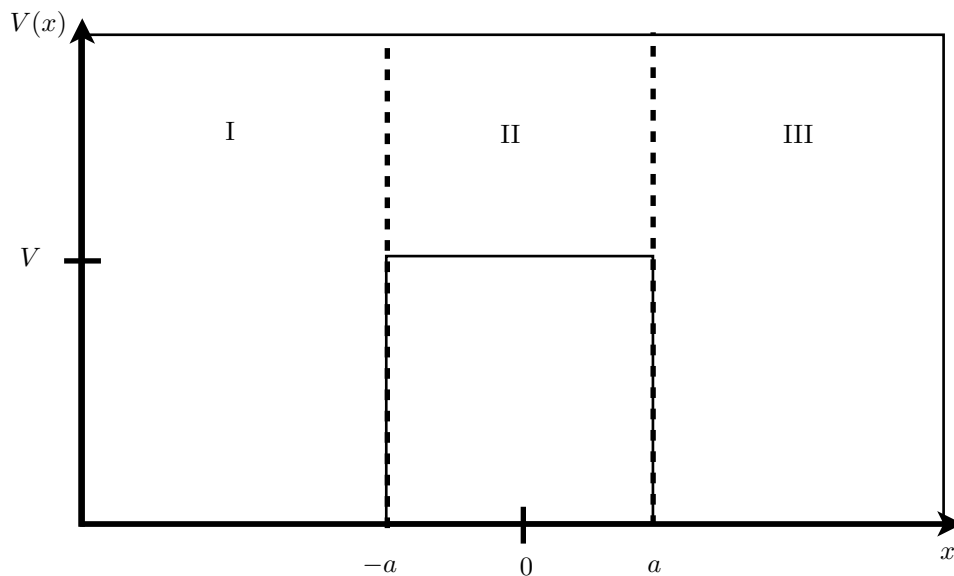


Figure 1: 1-D Scattering Potential

Alternatively, we may use the less clear S -matrix:

$$\begin{pmatrix} A_{\text{out}} \\ B_{\text{out}} \end{pmatrix} = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix} \begin{pmatrix} A_{\text{in}} \\ B_{\text{in}} \end{pmatrix}$$

The system obeys an equation of continuity (probability conservation):

$$\partial_t |\psi|^2 + \partial_x J = 0$$

where

$$J = \frac{\hbar}{m} \text{Im}(\psi^* \partial_x \psi)$$

The currents in regions I and III gives

$$J_I = \frac{\hbar k}{m} [|A_{\text{in}}|^2 - |A_{\text{out}}|^2]$$

$$J_{III} = \frac{\hbar k}{m} [|B_{\text{out}}|^2 - |B_{\text{in}}|^2]$$

The equation of continuity then tells us that

$$|A_{\text{out}}|^2 + |B_{\text{out}}|^2 = |A_{\text{in}}|^2 + |B_{\text{in}}|^2$$

$$\begin{pmatrix} A_{\text{out}}^* & B_{\text{out}}^* \end{pmatrix} \begin{pmatrix} A_{\text{out}} \\ A_{\text{out}} \end{pmatrix} = \begin{pmatrix} A_{\text{in}}^* & B_{\text{in}}^* \end{pmatrix} S^\dagger S \begin{pmatrix} A_{\text{in}} \\ B_{\text{in}} \end{pmatrix}$$

For scattering states, we let $B_{\text{in}} = 0$, that is, particles are *only* incident from the left. Then we have

$$\psi_k(x) = \begin{cases} A_{\text{in}} e^{ikx} + A_{\text{out}} e^{-ikx} & x < -a \\ B_{\text{out}} e^{ikx} & x > a \end{cases}$$

and we have

$$B_{\text{out}} = S_{21} A_{\text{in}}$$

$$A_{\text{out}} = S_{11} A_{\text{in}}$$

We define transmission and reflection coefficients

$$T \equiv \frac{|B_{\text{out}}|^2}{|A_{\text{in}}|^2} = |S_{21}|^2$$

$$R \equiv \frac{|A_{\text{out}}|^2}{|A_{\text{in}}|^2} = |S_{11}|^2$$

Landauer Formula

$$G = \frac{I}{V} \Rightarrow G = \frac{e^2}{h} T$$

where e^2/h is the quantum of conductance.

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Derivation of the Landauer Formula

Suppose we send in a wave with wave number k and energy $E = \hbar^2 k^2 / 2m$ from the left. As expected, we would get a portion of the wave to be reflected (proportional to S_{11}) the remainder to be transmitted (proportional to S_{21}).

The Scattering State is then given by

$$\psi_1^k(x) = \begin{cases} \frac{e^{i\phi_1 k}}{\sqrt{2\pi}} (e^{ikx} + S_{11}e^{-ikx}) & x < -a \\ \frac{e^{i\phi_1 k}}{\sqrt{2\pi}} S_{21}e^{ikx} & x > a \end{cases}$$

$$\psi_2^k(x) = \begin{cases} \frac{e^{i\phi_2 k}}{\sqrt{2\pi}} (e^{ikx} + S_{22}e^{-ikx}) & x > a \\ \frac{e^{i\phi_2 k}}{\sqrt{2\pi}} S_{12}e^{-ikx} & x < -a \end{cases}$$

With this, we are ready to...

For $T = 0$, we have incident electrons up to chemical potential μ . On different leads on a quantum wire, we generally have two different chemical potentials, which causes a net transport of electrons. Suppose on the left we have μ_1 and on the right we have μ_2 with $\mu_1 < \mu_2$, which causes an electrical net current from left to right. Our goal is to study this current in terms of the S -matrix.

Fermi Wave Number We define the Fermi Wave Number by

$$k_F = \frac{1}{\hbar} \sqrt{2m\mu}$$

The probability current for e^{-1} at k is given by

$$J_j^k = \frac{\hbar}{m} \text{Im} [\psi_j^{k*}(x) \partial_x \psi_j^k(x)]$$

The electrical current is then

$$I|_{x>a} = eJ_j^k = e \frac{\hbar}{m} \left[\int_0^{k_{F_1}} dk \frac{k}{2\pi} |S_{21}|^2 + \int_0^{k_{F_2}} dk \frac{k}{2\pi} (-1 + |S_{22}|^2) \right]$$

Then the transmission probability if $T_k \equiv |S_{21}|^2$, which gives the current to be

$$I = \frac{e}{2\pi} \int_{k_{F_2}}^{k_{F_1}} dk \left(\frac{\hbar k}{m} \right) T_k = \frac{3}{2\pi\hbar} \int_{\mu_2}^{\mu_1} dE T(E)$$

Where we have used $E = \hbar^2 k^2 / 2m$ and $dE = (\hbar^2 k / m) dk$. We may relate the two chemical potentials to the electric voltage via

$$\mu_1 = \mu_2 + eV$$

Linear Response The conductance is given by

$$G = \lim_{V \rightarrow 0} \frac{I}{V}$$

Then the electric current can be rewritten as

$$I = \frac{e}{2\pi\hbar} \int_{\mu_2}^{\mu_2 + eV} dE T(e) = \frac{e^2}{h} T(\mu) V$$

and then the conductance in this linear response limit is

$$G = \frac{I}{V} = \frac{e^2}{h} T(\mu) = \frac{e^2}{h} T(E_F)$$

1.3.3 Some Comments

1. Suppose we have a perfect wire with *no* backscattering. That is, $T = 1$. Then we have $R = \frac{1}{G} = 0$. This would of course be superconductivity.
2. This theory can be generalized to multichannel wires with many leads. The resulting conductance for N leads is then

$$G = \frac{e^2}{h} 2N$$

where the factor of 2 comes from electron spin degeneracy.

3. This theory has been validated by experiment with a quantum wire circuit setup that revealed a stair-step plot of conductance as a function of input voltage.
4. We have ignored the fact that the electrons interact and experience interactions off of one another (calculations effectively carried out at zero temperature). As a result, these resistances do not necessarily add in series.

1.4 Inelastic Scattering

In the field of inelastic scattering, we typically consider the situation of a particle scattering off of a quantum mechanical system. This system could be a liquid, a solid, a nuclei... anything, really. The inelastic condition implies that the act of scattering transfers energy between the particle and the target.

1.4.1 Setup and Notation

To ease the theory, we will suppose that the “target” will be composed of particles with position operators \mathbf{R}_i and momentum operators \mathbf{P}_i . The incident particle will have position operator \mathbf{R} and \mathbf{P} . The Hamiltonian of the system will be

$$\hat{\mathcal{H}} = \frac{\mathbf{P}^2}{2m} + \hat{H} + V$$

Where the first term is the kinetic energy of the particle, the non-script Hamiltonian is the internal energy of the target (kinetic plus potential), and the term V is the interaction potential. To simplify the system, we shall assume that the interaction potential takes on the form

$$V = \sum_{i=1}^N V(\mathbf{R} - \mathbf{R}_i)$$

Density Operator It becomes useful to define a density operator for the target. It is

$$\rho(\mathbf{r}) = \sum_{i=1}^N \delta^3(\mathbf{r} - \mathbf{R}_i)$$

where \mathbf{r} is simply a c-number position coordinate (multiplied by identity). We will use the Fourier transform of this operator,

$$\rho(\mathbf{q}) = \int d^3\mathbf{r} e^{-i\mathbf{q}\cdot\mathbf{r}} \rho(\mathbf{r}) = \sum_{i=1}^N e^{-i\mathbf{q}\cdot\mathbf{R}_i}$$

Rewriting the Interaction Potential This density operator can help us rewrite the potential into a more useful form:

$$V = \sum_{i=1}^N \int \frac{d^3\mathbf{q}}{(2\pi)^3} V(\mathbf{q}) e^{i\mathbf{q}\cdot(\mathbf{R}-\mathbf{R}_i)} = \int \frac{d^3\mathbf{q}}{(2\pi)^3} V(\mathbf{q}) \rho(\mathbf{q}) e^{i\mathbf{q}\cdot\mathbf{R}} \quad (1)$$

which is just the definition of the Fourier Transform of the interaction potential in the first line, and then a re-expression in terms of the density operator in the second line.

1.4.2 Modeling Scattering

Fermi's Golden Rule Suppose we start with an initial state $|\mathbf{k}; E_i, \alpha\rangle$, where \mathbf{k} is the wavevector of the incoming particle, E_i is the initial internal energy of the target and α indexes the particular state with energy E (since there may be degeneracy). If we end with a final state $|\mathbf{k}'; E_f, \beta\rangle$, then Fermi's Golden Rule tells us

$$\Gamma_{i \rightarrow f} = \frac{2\pi}{\hbar} |\langle \mathbf{k}'; E_f, \beta | V | \mathbf{k}; E_i, \alpha \rangle|^2 \delta(E_f + \epsilon_{k'} - E_i - \epsilon_k)$$

Where the delta function maintains energy conservation (fuck you Bill). For brevity, we'll denote the matrix element as V_{fi} . In terms of the interaction potential, this matrix element is then, using equation 1,

$$V_{fi} = \int \frac{d^3\mathbf{q}}{(2\pi)^3} V(\mathbf{q}) \langle \mathbf{k}'; E_f, \beta | \rho(\mathbf{q}) e^{i\mathbf{q}\cdot\mathbf{R}} | \mathbf{k}; E_i, \alpha \rangle \quad (2)$$

We now make use of the fact that the momentum and position operators are conjugate operators:

$$e^{ia\hat{p}/\hbar} |x\rangle = |x+a\rangle$$

$$e^{iq\hat{x}} |k\rangle = |k+q\rangle$$

So now we have

$$e^{i\mathbf{q}\cdot\mathbf{R}} |\mathbf{k}\rangle = |\mathbf{k} + \mathbf{q}\rangle$$

Now, the state ket we have written is really a direct product,

$$|\mathbf{k}; E_i, \alpha\rangle = |\mathbf{k}\rangle \otimes |E_i, \alpha\rangle. \quad (3)$$

Since \mathbf{R} only acts on the portion of the direct product pertaining to the incoming particle, and $\rho(\mathbf{q})$ only acts on the portion of the direct product pertaining to the target, we can write,

$$\langle \mathbf{k}'; E_f, \beta | \rho(\mathbf{q}) e^{i\mathbf{q}\cdot\mathbf{R}} | \mathbf{k}; E_i, \alpha \rangle = \langle E_f, \beta | \rho(\mathbf{q}) | E_i, \alpha \rangle \langle \mathbf{k}' | e^{i\mathbf{q}\cdot\mathbf{R}} | \mathbf{k} \rangle \quad (4)$$

$$= \langle E_f, \beta | \rho(\mathbf{q}) | E_i, \alpha \rangle \langle \mathbf{k}' | \mathbf{k} + \mathbf{q} \rangle = \langle E_f \beta | \rho(\mathbf{q}) | E_i \alpha \rangle \delta^3(\mathbf{k}' - \mathbf{k} - \mathbf{q}) \quad (5)$$

Thus the matrix element can be written as, using equations 2, 4 and 5,

$$V_{fi} = \frac{V(\mathbf{k}' - \mathbf{k})}{(2\pi)^3} \langle E_f \beta | \rho(\mathbf{k}' - \mathbf{k}) | E_i \alpha \rangle$$

Now we are interested in calculating the differential cross-section, which is

$$\left(\frac{d^2\sigma}{d\epsilon d\Omega} \right) d\Omega d\epsilon \equiv \frac{\# \text{ of scattered particles/time into solid angle } d\Omega \text{ and energy } \epsilon \rightarrow \epsilon + d\epsilon}{\# \text{ of incident particles/time-area}}$$

Then using Fermi's Golden Rule,

$$\Gamma_{i \rightarrow d\Omega d\epsilon} = \Gamma_{i \rightarrow f} k'^2 dk' d\Omega = \Gamma_{i \rightarrow f} \left(\frac{m}{\hbar^2} \right) k' d\epsilon d\Omega$$

With

$$\epsilon = \frac{\hbar^2 k'^2}{2m} \Rightarrow d\epsilon = \frac{\hbar^2}{m} k' dk'$$

The differential cross section is now

$$\frac{d^2\sigma}{d\Omega d\epsilon} = \frac{\sum_{E_f, \beta} \left(\frac{m}{\hbar^2} \right) k' \Gamma_{i \rightarrow f}}{\left(\frac{1}{2\pi} \right)^3 \left(\frac{\hbar k}{m} \right)} = \left(\frac{m}{2\pi \hbar^2} \right)^2 |V(\mathbf{k}' - \mathbf{k})|^2 \frac{k'}{k} \sum_{E_f, \beta} \delta(E_f + \epsilon_{k'} - E_i - \epsilon_k) |\langle E_f \beta | \rho(\mathbf{k}' - \mathbf{k}) | E_i \alpha \rangle|^2$$

Dynamical Structure Factor To simplify the form of the cross-section, we introduce the dynamical structure factor (DSF), defined as

$$S(\mathbf{q}, \omega) = \sum_{E_f, \beta} \delta \left(\omega + \frac{E_f - E_i}{\hbar} \right) |\langle E_f \beta | \rho(\mathbf{q}) | E_i \alpha \rangle|^2$$

where the DSF pertains only to the *target*, and for now ω is just a parameter. In terms of the DSF, we can write the cross-section as

$$\frac{d^2\sigma}{d\Omega d\epsilon} = \left(\frac{m}{2\pi \hbar^2} \right)^2 |V(\mathbf{k}' - \mathbf{k})|^2 \frac{k'}{k} S(\mathbf{q}, \epsilon_{k'} - \epsilon_k). \quad (6)$$

where we are careful to note that the term V which appears is the Fourier transform of the potential. We now want to find a way to simplify the expression for the DSF. Rewriting the delta function,

$$S(\mathbf{q}, \omega) = \sum_{E_f, \beta} \int dt e^{i\omega t} e^{i(E_f - E_i)t/\hbar} \langle E_i \alpha | \rho(-\mathbf{q}) | E_f \beta \rangle \langle E_f \beta | \rho(\mathbf{q}) | E_i \alpha \rangle \quad (7)$$

which can be further simplified by noting that, since the kets are energy eigenstates,

$$e^{it(E_f - E_i)/\hbar} \langle E_f \beta | \rho(\mathbf{q}) | E_i \alpha \rangle = \left\langle E_f \beta \left| e^{iHt/\hbar} \rho(\mathbf{q}) e^{-iHt/\hbar} \right| E_i \alpha \right\rangle \quad (8)$$

So the dynamical structure factor is then

$$S(\mathbf{q}, \omega) = \sum_{E_f \beta} \int dt e^{i\omega t} \langle E_i \alpha | \rho(-\mathbf{q}) | E_f \beta \rangle \left\langle E_f \beta \left| e^{iHt/\hbar} \rho(\mathbf{q}) e^{-iHt/\hbar} \right| E_i \alpha \right\rangle \quad (9)$$

Since we now see we have a completeness relation, we can perform the summation to get

$$S(\mathbf{q}, \omega) = \int \frac{dt}{2\pi} e^{i\omega t} \langle E_i \alpha | \rho(-\mathbf{q}, 0) \rho(\mathbf{q}, t) | E_i \alpha \rangle, \quad (10)$$

which is a particularly useful form since it involves the expectation value of some operator in the initial state of the target particle. Equations 6 and 10 are the results we will most often want to use (in particular for HW1 P3!). Note that $\rho(\mathbf{q}, t)$ is just the second operator sandwiched in equation 9, which corresponds to the usual Heisenberg picture definition.

Thermal Targets For a thermodynamic situation with the target at some temperature T , for some operator $\hat{\theta}$,

$$\langle \hat{\theta} \rangle \equiv \frac{1}{Z} \sum_{E, \alpha} e^{-\beta E} \langle E_\alpha | \hat{\theta} | E_\alpha \rangle; \quad Z = \sum_{E, \alpha} e^{-\beta E}$$

$$S(\mathbf{q}, \omega) = \int \frac{dt}{2\pi} e^{i\omega t} \langle \rho(-\mathbf{q}, 0) \rho(\mathbf{q}, t) \rangle$$

Some Comments

1. If we don't measure the final energy (i.e. we measure the *direction*),

$$S_{\text{static}}(\mathbf{q}) = \int d\omega S(\mathbf{q}, \omega) = \langle \rho(-\mathbf{q}) \rho(\mathbf{q}) \rangle = \left\langle \left| \sum_i e^{-\mathbf{q} \cdot \mathbf{R}_i} \right|^2 \right\rangle$$

2. If the target particles are very heavy (i.e. they do not move),

$$\rho(\mathbf{q}, t) = \rho(\mathbf{q})$$

and

$$S(\mathbf{q}, \omega) = S(\omega) S_{\text{static}}(\mathbf{q})$$

3. (MISSING IMPORTANT FIGURE)

For particles traveling with a path length difference, a phase difference is accumulated:

$$\Delta\phi_i = \frac{2\pi}{\lambda} \hat{R}_i \hat{k} - \frac{2\pi}{\lambda'} \hat{R}_i \hat{k}' = \mathbf{R}_i \cdot (\mathbf{k} - \mathbf{k}') = -\mathbf{R}_i \cdot \mathbf{q}$$

$$\text{Amp} \approx \sum_i e^{i\Delta\phi_i} \cong \sum_i e^{-i\mathbf{q} \cdot \mathbf{R}_i} = \rho(\mathbf{q})$$

So the scattered intensity is

$$S(\mathbf{q}) \sim \langle |\text{Amp}| \rangle = \langle \rho(\mathbf{q}) \rho(-\mathbf{q}) \rangle$$

1.4.3 Scattering Examples

Suppose we scatter off of a solid or liquid with length scale $a \sim 3\text{\AA}$ and energy scale $k_B T_{\text{room}} \sim 300\text{ K}$.

Light Scattering

$$\epsilon = \hbar\omega = \hbar ck = \frac{hc}{\lambda} \approx 10^4 \text{ eV} \sim 10^7 \text{ K}$$
$$\Delta\epsilon \sim 300 \text{ K}$$

This is in fact X-Ray scattering.