Greens function Approach to Transport: Basic Training in Condensed Matter Physics

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Lecture Notes: Spring 2018

Preface

About Basic Training

Basic Training in Condensed Matter physics is a modular team taught course offered by the theorists in the Cornell Physics department. It is designed to expose our graduate students to a broad range of topics. Each module runs 2-4 weeks, and require a range of preparations. This module, "Greens Function Approach to Transport," is designed for students who have completed a standard one semester graduate solid state physics course. It assumes no prior exposure to many-body Greens functions, but requires a knowledge of second quantization.

Prior Topics

2006 Random Matrix Theory (Piet Brouwer)
Quantized Hall Effect (Chris Henley)
Disordered Systems, Computational Complexity, and Information Theory (James Sethna)
Asymptotic Methods (Veit Elser)

2007 Superfluidity in Bose and Fermi Systems (Erich Mueller)
Applications of Many-Body Theory (Tomas Arias)
Rigidity (James Sethna)
Asymptotic Analysis for Differential Equations (Veit Elser)

2008 Constrained Problems (Veit Elser)
Quantum Optics (Erich Mueller)
Quantum Antiferromagnets (Chris Henley)
Luttinger Liquids (Piet Brouwer)

2009 Continuum Theories of Crystal Defects (James Sethna)
Probes of Cold Atoms (Erich Mueller)
Competing Ferroic Orders: the Magnetoelectric Effect (Craig Fennie)
Quantum Criticality (Eun-Ah Kim)

2010 Equation of Motion Approach to Many-Body Physics (Erich Mueller)
Dynamics of Infectious Diseases (Chris Myers)
The Theory of Density Functional Theory: Electronic, Liquid, and Joint (Tomas Arias)
Nonlinear Fits to Data: Sloppiness, Differential Geometry and Algorithms (James Sethna)

2011 Practical Density Functional Theory (Tomas Arias)
Semiclassical Methods (Erich Mueller)
Ginzburg-Landau Theory of Superconductivity (Chris Henley)
Continuum Quantum Monte Carlo Methods in Chemistry and Physics (Cyrus Umrigar)

2012 Quantum 14-15 puzzle: mechanics of a single hole in a spin-1/2 lattice (Veit Elser)
The science of writing Science (Eun-Ah Kim)
Feynman diagrams and *ab-initio* computation of excited states in condensed matter (Tomas Arias)
Probes of Cuprate Superconductors (theorist's view) (Chris Henley)
Physics of Life (Jane Wang)

2013 Many Body Field Theory (Erich Mueller)
The Theory of Density Functional Theory: Electronic, Liquid, and Joint (Tomas Arias)
Conformal Symmetry (Andre Leclair)
Nonlinear Fits to Data: Sloppiness, Differential Geometry and Algorithms (James Sethna)

2014 Rigidity (James Sethna)
Practical Density Functional Theory (Tomas Arias)
Quantum Monte-Carlo (Cyrus Umrigar)
Geometry in Quantum Mechanics (Erich Mueller)

2018 Greens Function approach to Transport (Erich Mueller)
Dynamical Systems that solve hard problems (Viet Elser)
Variational and Projector Monte Carlo Methods for Physics and Chemistry (Cyrus Umrigar)
Sloppy Models (Jim Sethna)

Contents

Chapter 1

Introduction – Jan 24, 2018

A. Logistics

I hate to start with logistics, but it is necessary. This is a modular course with three long modules, and one short. To get credit, you need to complete two of the three long modules – including the homework. If you want to audit the course, you are welcome. It helps us out if you officially sign-up to audit, rather than just show up.

I expect that there will be some students attending class who are not signed up. You are welcome to do so. I will send around a sign-up sheet so that I have everyone's email address. If you did not sign up, I would appreciate a quick email, so that I can add you to the list.

Due to various obligations, there are two classes that I will have to cancel: Jan 26 and Feb 14. I would like to schedule make-up classes. I will set up an electronic poll once I have everyone's email addresses.

Each module is structured in a unique way. I am going to be giving homework problems every class. You will have one week to complete them. They should not be too heavy. You can get a feel for the scope by looking at the web site.

Over the past few years I have discovered that I don't like writing equations on the board. Thus my lectures will be structured so that you mostly figure the math out yourself. I will post my lectures the day before class – with the in-class questions included. I will hand out print-outs of the questions at the beginning of class, and will incorporate them into the lectures. After class I will post a copy of the notes with the answers to the problems.

B. Classical (Drude) Theory of Resistivity

Here are some problems (which we will go through in class) to remind you of the Drude theory of resistivity:

Problem 1.1. Classical Theory of Resistivity In the simplest model of resistivity one considers the motion of a particle with charge q and mass m being accelerated by an electric field of strength E in the $\hat{\mathbf{x}}$ direction.

1.1.1. Suppose the particle is moving at velocity $\tilde{\mathbf{v}}_\mathbf{0}$ at time $t = 0$, what will its velocity be at time t?

Solution 1.1.1. The force on the particle is $\tilde{\mathbf{F}} = qE\hat{\mathbf{x}}$, so Newton's laws read

$$m\frac{\partial \mathbf{v}}{\partial t} = qE\hat{\mathbf{x}}, \tag{1.1}$$

which implies

$$\tilde{\mathbf{v}} = \tilde{\mathbf{v}}_\mathbf{0} + \frac{qEt}{m}\hat{\mathbf{x}}. \tag{1.2}$$

1.1.2. Suppose after time τ, the particle bounces off something (a phonon, an impurity...) and its velocity resets in some random manner. That is initially the particle has velocity $\mathbf{v_0}$, the particle accelerates for a time τ, then it scatters off something and $\mathbf{v}$ becomes $\mathbf{v_1}$. It again accelerates for a time τ, then it again scatters, and $\mathbf{v}$ resets to $\mathbf{v_2}$. The velocities $\mathbf{v_j}$ are drawn from some set distribution, with zero mean.

What will the average velocity of the particle be?

Solution 1.1.2.

$$\langle\tilde{\mathbf{v}}\rangle = \langle\tilde{\mathbf{v}}_\mathbf{j}\rangle + \frac{qE\tau}{2m}\hat{\mathbf{x}} \tag{1.3}$$

$$= \frac{qE\tau}{2m}\hat{\mathbf{x}} \tag{1.4}$$

1.1.3. If the density of particles is n, what is the electrical current $\vec{j}$?

Solution 1.1.3.

$$\vec{j} = qn\vec{v} = \frac{q^2nEt}{2m}\hat{\mathbf{x}}. \tag{1.5}$$

1.1.4. Suppose we make a device out of this material, with length L, and cross-sectional area A. What will its resistance be?

Solution 1.1.4. The total current going through the device is jA. The total voltage drop is EL, thus the resistance is

$$R = \frac{V}{I} = \frac{EL}{jA} = \frac{2m}{q^2n\tau}\frac{L}{A} \tag{1.6}$$

B.1. Discussion

If you had a good solid state physics class you should know a few refinements to this argument. First, it is ridiculous to think that after every time τ there is a collision. Of course, the argument does not really depend on this. Instead, it suffices that the "reset" processes happen randomly, with a mean time between them of τ. We call τ the mean-free time. We call $v_d = qnE\tau/2m$ the "drift velocity". The drift velocity is typically quite small. In particular, it is much smaller than the rms velocity of a particle $\bar{v} = \sqrt{\langle v^2 \rangle}$ – which classically is the thermal velocity, but quantum mechanically is some fraction of the Fermi velocity. One often refers to the "mean free path", $\lambda = \bar{v}\tau$, which is typically interpreted as $\lambda = 1/(n_s\sigma)$, where n_s is the density of scatterers, and σ is the cross-section for scattering off the impurities.

The other refinement is that electrons in metals behave like they are heavier than electrons in free space. Thus one should replace m with m^*, the effective mass. The density of electrons n should also be replaced by the density of mobile electrons: For example, in an undoped semi-conductor, the only mobile electrons are those which are thermally excited into the conduction band, and hence $n \propto e^{-\Delta/k_B T}$, where Δ is the band-gap.

On further thought, maybe the carriers should not be electrons, but "quasi-particles" – some sort of collective excitation which acts like particles?

Regardless, I don't think I know how to use the Drude theory to actually calculate resistivity. In the homework we will go backwards – starting with measured data infer the parameters of the Drude theory.

C. Quantized Conductance (Landauer)

There is a completely different argument about resistivity which sometimes makes it into a solid-state physics course. It has the advantage of being quantum mechanical. It involves thinking about a very clean, very thin wire. So thin in fact that the electrons in it can be modeled via a 1D Schrodinger equation.

One imagines that far to the left, and far to the right, are leads. The electrons that are moving to the right must have come from the left lead – and those moving to the left must have come from the right lead.

Problem 1.2. Quantized Conductance

1.2.1. Consider the right-moving electrons in a 1D wire. They have all come from the left lead, so the occupation of a right-moving mode with wave-vector k will be

$$f_k^+ = \frac{1}{e^{\beta_L(\epsilon_k - \mu_L)} + 1}, \tag{1.7}$$

where β_L and μ_L are the inverse temperature and the chemical potential of the left lead. The dispersion relationship ϵ_k relates the energy and momentum. Here we will consider zero temperature, so

$$f_k^+ = \theta(\mu_L - \epsilon_k). \tag{1.8}$$

Use this expression to formally write the contribution to the current from the right-moving particles I_+ as an integral over k, with k running from 0 to k_f^L, where $\epsilon_{k_f^L} = \mu_L$. Assume that there are n_s degenerate spin states. [In most physical situations, $n_s = 2$.]

Solution 1.2.1.

$$I_+ = n_s q \int_{k>0} \frac{dk}{2\pi\hbar} \partial_k \epsilon_k f_k^+ \tag{1.9}$$

$$= \frac{q n_s}{2\pi\hbar} \int_0^{k_f^L} dk \partial_k \epsilon_k. \tag{1.10}$$

1.2.2. Do the integral – hint: what is the integral of a derivative?

Solution 1.2.2.

$$I_+ = \frac{q n_s}{2\pi\hbar} \mu_L. \tag{1.11}$$

1.2.3. What is the contribution to the current I_- from the left-moving particles?

Solution 1.2.3. By symmetry

$$I_- = -\frac{q n_s}{2\pi\hbar} \mu_R. \tag{1.12}$$

1.2.4. What is the net current?

Solution 1.2.4.

$$I = I_+ + I_- = \frac{q n_s}{2\pi\hbar} (\mu_L - \mu_R). \tag{1.13}$$

1.2.5. Finally we identify $qV = \mu_L - \mu_R$ as the voltage difference between the leads. What is the conductance $G = 1/R = I/V$?

Solution 1.2.5.

$$G = \frac{q^2 n_s}{2\pi\hbar} \tag{1.14}$$

C.1. Discussion

This result is quite peculiar, and completely unlike the Drude argument. Here we have no forces on the electrons, and no scattering. The resistance is independent of the length of the wire – which is unlike any ordinary macroscopic material.

The standard understanding is that this Landauer result is correct when the device is much smaller than the mean-free path. It should be understood as a *maximum* possible conductivity. Any sources of scattering will decrease the conductivity of the device.

The absence of forces is due to charging effects: one applies a potential difference between two reservoirs. The densities of electrons in each reservoir adjusts so that there are no forces.

One crucial generalization of this argument is to note that for a real wire there will be multiple independent 1D channels corresponding to the different transverse wavefunction of the electrons. Depending on the chemical potentials of the contacts, some number of these channels will be active, and the observed conductivity will be an integer multiple of the number we calculated in this lecture.

Our strategy in this course will be to generalize this Landauer result to more complicated geometries, and add both elastic and inelastic scattering processes.

An interesting note is that while quantized conductance can be observed in 1D wires (such as graphene nano-tubes), the simplest setting to see this physics is actually "point-contact." That is, imagine the left and right reservoir just touch at a single point. All of the electrons approaching the point from the left will enter the right reservoir. All of the electrons approaching the point from the right will enter the left reservoir. The arguments from lecture imply that the conductivity of the contact will be $G_0 = \frac{2e^2}{h}$. In the PHYS 6510 lab there is an experiment where you observe this phenomenon by simply placing two small gold wires on top of one-another. One then taps the table. As the wires jump, the contact will transiently open and close, and you will see this universal quantized conductance for a few ms. See: `http://pages.physics.cornell.edu/p510/E-16_Conductance_Quantization`.

D. Plan

I can now lay out the basic physics that we will use to model the conductivity of a device. The idea is cleanest if I first consider only elastic scattering.

As illustrated in Fig. 1.1, we will consider a generic device with several leads. The device contains various impurities or other defects which can lead to

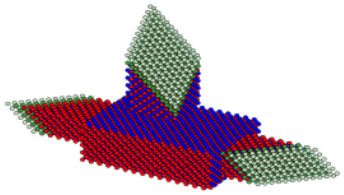


Figure 1.1: Schematic of device with 3 leads. Given voltages applied to each lead, we wish to calculate the currents.

(elastic) scattering. Each lead is attached to an infinite reservoir.

We imagine solving for the eigenstates of the entire system (reservoirs+leads+device). Some eigenstates correspond to bound states that do not extend into the leads. These do not contribute to transport. All other eigenstates can be chosen so that each one originates in a single lead. In the simple wire example of Sec. C, these are the left-moving and right-moving states. We occupy each eigenstate according to the chemical potential of the lead from which it originates. One can then calculate the currents by summing up the contribution from all of these states.

Of course, the challenge is that there are an infinite number of eigenstates. Luckily there are tools which allow us to calculate the net currents, without explicitly finding all of the eigenstates. This course is focussed on developing those tools. We will then generalize these arguments to include inelastic scattering.

E. Homework: Due Jan 31

Problem 1.3. Typical scales

1.3.1. The copper wire in your house is either 14 gauge or 12 gauge (depending on if it is a 15 Amp or 20 Amp circuit). A 12 gauge wire has a diameter of roughly 2 mm. If you drive a current of $I = 1A$ through one of these wires, roughly what would one expect the drift velocity to be? [You will need to estimate the electron density. There is roughly one conduction electron per nucleus.]

Solution 1.3.1. The current should be $I = qnvA$, or

$$v = \frac{I}{qnA} \tag{1.15}$$

The lattice constant of most crystals is of order a few Angstrom. Thus the electron density of copper should by somewhere in the neighborhood of $n \sim 10^{29} m^{-3}$. Thus the drift velocity is something like

$$\begin{aligned} v &\sim \frac{1A}{(1.610^{-19}C)(10^{29}m^{-3})(\pi 10^{-6}m^2)} && (1.16)\\ &\sim 10^{-5} m/s. && (1.17) \end{aligned}$$

1.3.2. Estimate the Fermi velocity in copper.

Solution 1.3.2. For a 3D degenerate Fermi gas, the density is related to the fermi velocity $v_f = k_f/m$ via

$$\begin{aligned} n &= \int_{|k|<k_f} \frac{d^3k}{(2\pi\hbar)^3} && (1.18)\\ &= \frac{(4/3)\pi k_f^3}{(2\pi\hbar)^3} && (1.19) \end{aligned}$$

In other words

$$\begin{aligned} v_f &= \frac{\hbar}{m}(6\pi^2 n)^{1/3} && (1.20)\\ &\approx 10^6 m/s. && (1.21) \end{aligned}$$

1.3.3. Is our assumption that the drift velocity is small compared to the Fermi velocity reasonable?

Solution 1.3.3. Very much so!

1.3.4. At room temperature the resistance of 1 meter of 12 gauge wire is roughly 5mΩ. Using the semiclassical transport theory, estimate the mean-free path?

Solution 1.3.4. According to the semiclassical theory, $R = 2mL/(q^2nA\tau)$. The mean free path is $\lambda = v_f\tau$, and hence

$$\lambda = \frac{2mv_fL}{RAq^2n} \tag{1.22}$$

$$\approx \frac{2(10^-30kg)(10^6m/s)(1m)}{(5\cdot 10^-3m/s)(\pi 10^{-6}m^2)(1.6\cdot 10^-19C)^2(10^{29}m^{-3})} \tag{1.23}$$

$$\approx 10^{-7}m. \tag{1.24}$$

To be honest I am not sure if this lengthscale actually means anything physical.

Problem 1.4. Density of states and currents Consider a 1D wire of length L with periodic boundary conditions and dispersion ϵ_k.

1.4.1. What is the normalized wavefunction of a particle with wave-vector k?

Solution 1.4.1.

$$\psi_k(x) = \frac{1}{\sqrt{L}}e^{ikx} \tag{1.25}$$

1.4.2. What are the allowed wave-vectors k?

Solution 1.4.2.

$$k = \frac{2\pi n}{L} \tag{1.26}$$

1.4.3. For a generic dispersion ϵ_k, what is the velocity of a particle with wave-vector k? [In other words, what is the group velocity of a wave-packet centered around wave-vector k.]

Solution 1.4.3. This is a standard wave-mechanics result,

$$v = \frac{1}{\hbar}\partial_k\epsilon_k. \tag{1.27}$$

1.4.4. What is the contribution to the current of a particle with wave-vector k?

Solution 1.4.4. Current is charge times velocity times density. The density of a particle in some k-state is $1/L$. So the contribution to the current is

$$j_k = \frac{e}{\hbar L}\partial_k\epsilon_k \tag{1.28}$$

1.4.5. If the state with wave-vector k is occupied with probability f_k, write sums which corresponds to the total density and total current. [Neglect Spin.]

Solution 1.4.5. The total density is

$$n = \frac{1}{L} \sum_{k=2\pi n/L} f_k. \tag{1.29}$$

The total current is

$$j = \frac{1}{\hbar L} \sum_{k=2\pi n/L} f_k \partial_k \epsilon_k \tag{1.30}$$

1.4.6. Take $L \to \infty$, and convert the sums into integrals.

Solution 1.4.6. The Riemann integral can be taken to be the limit

$$\int ds\, G(s) = \lim_{\delta \to 0} \sum_{s=n\delta} \delta G(s). \tag{1.31}$$

In our case $\delta = 2\pi/L$, and the integrals are

$$n = \int \frac{dk}{2\pi} f(k) \tag{1.32}$$

$$j = \frac{e}{\hbar} \int \frac{dk}{2\pi} f(k) \partial_k \epsilon_k. \tag{1.33}$$

It is not part of the question, but one can typically write $f(k) = f_+(\epsilon_k)$ for $k > 0$ and $f(k) = f_-(\epsilon_k)$ for $k < 0$. One then finds

$$j = \frac{e}{\hbar} \int \frac{d\epsilon}{2\pi} (f_+(\epsilon) - f_-(\epsilon)). \tag{1.34}$$

At zero temperature this gives the quantized Landauer conductivity.

Problem 1.5. Transmission and Reflection Consider a 1D wire, with an impurity which can be modeled as a potential $V(r) = V_0 \delta(r)$. As you learned in your quantum mechanics class, for $V_0 > 0$, a complete set of eigenstates of the Schrodinger equation can be drawn from two classes: those which are incident from the left, and those which are incident from the right. That is, if we let $k > 0$ we can find eigenstates of the form

$$\psi_+(x) = \theta(-x) \left[e^{ikx} + t_{11}(k) e^{-ikx} \right] + \theta(x) t_{12}(k) e^{ikx} \tag{1.35}$$

$$\psi_-(x) = \theta(x) \left[e^{-ikx} + t_{22}(k) e^{ikx} \right] + \theta(-x) t_{21}(k) e^{-ikx}, \tag{1.36}$$

where $t_{ij}(k)$ are found by satisfying the matching conditions at the origin:

$$\psi(0^+) = \psi(0^-) \tag{1.37}$$

$$\left. \frac{\psi'(x)}{\psi(x)} \right|_{0^-}^{0^+} = 2mV_0/\hbar^2. \tag{1.38}$$

Note: I will not have you solve these equations – if you have never done it before it is good for your soul (only takes a few lines). It suffices to know that if we wanted to we could calculate the coefficients $t_{ij}(k)$.

These states in Eq. (1.35) have energy $E = \hbar^2 k^2/2m$. Neglect spin.

1.5.1. Suppose you know the transmission amplitudes $t_{ij}(k)$. Further suppose that all states originating on the left with energy $E < \mu_1$ are occupied, and all state originating on the right with energy $E < \mu_2$ are occupied. What is the net current going from the left lead to the right lead in terms of integrals over the $t_{ij}(k)$? Hint: The measure for the integral is far from obvious, but in the reflectionless limit the result should reduce to that in problem 1.4. In future lectures we will develop a more systematic approach.

Note: in complete generality $|t_{12}| = |t_{21}|$.

Solution 1.5.1. The current from left to right should be

$$j_+ = \frac{e}{\hbar}\int_{E_k<\mu_1} \frac{dk}{2\pi}(\partial_k E_k)|t_{12}(k)|^2 \tag{1.39}$$

$$= \frac{e}{\hbar}\int^{\mu_1} \frac{d\epsilon}{2\pi}|t_{12}(\epsilon)|^2. \tag{1.40}$$

Conversely, the current from right to left should be

$$j_- = \frac{e}{\hbar}\int_{E_k<\mu_2} \frac{dk}{2\pi}(\partial_k E_k)|t_{21}(k)|^2 \tag{1.41}$$

$$= \frac{e}{\hbar}\int^{\mu_2} \frac{d\epsilon}{2\pi}|t_{12}(\epsilon)|^2. \tag{1.42}$$

Thus the total current is

$$j = \frac{e}{\hbar}\int_{\mu_1}^{\mu_2} \frac{d\epsilon}{2\pi}|t_{12}(\epsilon)|^2 \tag{1.43}$$

1.5.2. Take $\mu_2 = \mu + V/2$ and $\mu_1 = \mu - V/2$. Write an expression for the conductivity $G = \partial I/\partial V$ evaluated at $V = 0$?

Solution 1.5.2. For small V, the current will be

$$j = \frac{e}{2\pi\hbar}V|t_{12}(\mu)|^2. \tag{1.44}$$

Thus the conductivity is

$$G = \frac{e}{2\pi\hbar}|t_{12}(\mu)|^2. \tag{1.45}$$

1.5.3. For $V_0 < 0$ there also exists an eigenstate of the Schrodinger equation which is neither incident from the left, nor from the right. What is it? Does it contribute to the current?

Solution 1.5.3. This extra solution is a bound state. It carries no current.

Chapter 2

Intro to Python/Kwant – date TBD

Our second class will be a computer lab where we go through a IPython Notebook which will teach you some computer basics that we will be using. Unless someone objects, we will run this as a "Bring Your Own Computer" lab.

A. Homework – Due date TBD

Complete the notebook.

Chapter 3

Open Quantum Systems – Jan 31, 2018

As explained last day, the way we will calculate transport is that we will model both our system, and the leads that are attached to it. Every eigenstate which contributes to the current can be taken to originate in one of the leads. We fill those states based on the chemical potential of the lead.

The problem is book-keeping. We have an infinite system with an infinite number of eigenstates. Today we will introduce a simple toy problem which will help us develop some of the needed machinery. This problem is the classic "decay of a single mode coupled to a continuum". In the transport context we will imagine that we have a small metallic grain – a quantum dot – which can hold a single electron. It is in close proximity to a large conductor, which provides a bath. We will imagine at time $t = 0$ we put an electron on the dot. We then want to calculate how it escapes.

It is convenient to use "second quantized" notation to describe this model. This notation is not necessary, but will make our life easier. If you need a refresher on this notation, there is a homework problem, and I would be happy to help you out.

We let $\hat{a}^\dagger$ denote the operator which adds a particle to the mode that is on the dot – and $\hat{a}$ is the operator that removes a particle from that mode. We will neglect spin, and $\hat{a}^\dagger\hat{a}$ is the operator which counts how many particles are on the dot. Similarly, we let $\hat{b}_j$ be the operator that removes a particle from the j'th mode of the reservoir. We will take the dot-mode to have energy ϵ_0, and the j'th reservoir mode to have energy ϵ_j. The Hamiltonian will be

$$H = \epsilon_0 \hat{a}^\dagger \hat{a} + \sum_j \epsilon_j \hat{b}_j^\dagger \hat{b}_j + \sum_j \lambda_j \hat{a}^\dagger \hat{b}_j + \lambda_j^* \hat{b}_j^\dagger \hat{a}. \tag{3.1}$$

Here λ_j parameterizes the coupling between the j'th reservoir mode and the dot mode.

A. Wave-function approach

We will first analyze this problem in an "elementary" manner – that is by writing down a wavefunction, and finding the differential equations obeyed by the coefficients. We will later develop more sophisticated language which is easier to generalize.

At time $t = 0$ we want to be in the state where the dot mode is occupied and all other modes are empty. This is conveniently written as

$$|t = 0\rangle = \hat{a}^\dagger|\text{vac}\rangle, \tag{3.2}$$

where $|\text{vac}\rangle$ is the state containing no particles. Our goal will be to follow the time-evolution of this state.

Note: this model might be more familiar in the context of atomic physics. We identify $\hat{a}^\dagger|\text{vac}\rangle$ with that of an excited atom. We further identify $\hat{b}_j^\dagger|\text{vac}\rangle$ with that of a ground-state atom in the presence of a photon which occupies the j'th mode of the electromagnetic field. Equation (3.4) then corresponds to the Hamiltonian one would use to calculate the decay of the atom into its ground-state.

We are going to take an "elementary" approach. Next day we will consider this problem using a bit more technology.

Problem 3.1. Decay into a continuum We wish to time evolve the state

$$|t = 0\rangle = \hat{a}^\dagger|\text{vac}\rangle, \tag{3.3}$$

under the Hamiltonian

$$H = \epsilon_0 \hat{a}^\dagger \hat{a} + \sum_j \epsilon_j \hat{b}_j^\dagger \hat{b}_j + \sum_j \lambda_j \hat{a}^\dagger \hat{b}_j + \lambda_j^* \hat{b}_j^\dagger \hat{a}. \tag{3.4}$$

3.1.1. The most general state we will have at time t is

$$|t\rangle = A(t)\hat{a}^\dagger|\text{vac}\rangle + \sum_j B_j(t)\hat{b}_j^\dagger|\text{vac}\rangle. \tag{3.5}$$

Use the Schrodinger equation

$$i\hbar\partial_t|t\rangle = H|t\rangle, \tag{3.6}$$

to derive equations of motion for the coefficients $A(t)$ and $B_j(t)$.

Solution 3.1.1. We plug the Ansatz of Eq. (3.5) into the time dependent Schrodinger equation to find

$$\left[i\hbar A'(t) + \sum_j i\hbar B_j'(t)\hat{b}_j^\dagger\right]|\text{vac}\rangle = \left[\epsilon_0 A(t) + \sum_j \lambda_j B_j(t)\right] a^\dagger|\text{vac}\rangle \quad (3.7)$$

$$+\sum_j \left[\epsilon_j B_j(t) + \lambda_j^* A(t)\right] b_j^\dagger|\text{vac}\rangle \quad (3.8)$$

Equating coefficients yields

$$i\hbar A'(t) = \epsilon_0 A(t) + \sum_j \lambda_j B_j(t) \quad (3.9)$$

$$i\hbar B_j'(t) = \epsilon_j B_j(t) + \lambda_j^* A(t). \quad (3.10)$$

3.1.2. We will solve these equations using the Laplace transform. That is we define $A(s)$ and $B_j(s)$ such that

$$A(s) = \int_0^\infty dt\, e^{-st} A(t) \quad (3.11)$$

and

$$B_j(s) = \int_0^\infty dt\, e^{-st} B_j(t). \quad (3.12)$$

Write an expression for

$$\bar{A}(s) = \int_0^\infty dt\, e^{-st} A'(t) \quad (3.13)$$

in terms of $A(s)$ and $A(t=0)$. Hint: Integrate by parts.

Solution 3.1.2.

$$\bar{A}(s) = \int_0^\infty dt e^{-st} A'(t) \quad (3.14)$$

$$= e^{-st}A(t)\big|_0^\infty + \int_0^\infty dt e^{-st} A(t) \quad (3.15)$$

$$= -A(t=0) + sA(s). \quad (3.16)$$

3.1.3. Multiply Eq. (3.35) by e^{-st} and integrate over time to derive a coupled set of equations for $A(s)$ and $B_j(s)$.

Solution 3.1.3.

$$(i\hbar s - \epsilon_0)A(s) - \sum_j \lambda_j B_j(s) = i\hbar \quad (3.17)$$

$$-\lambda_j^* A(s) + (i\hbar s - \epsilon_j)B_j(s) = 0. \quad (3.18)$$

3.1.4. The coefficients of the bath modes can be eliminated to write

$$(i\hbar s - \epsilon_0 - \Sigma(is))A(s) = i\hbar. \tag{3.19}$$

Find the function $\Sigma(is)$. This function is referred to as the "self-energy." It encodes all information about how the environment influences the dot.

Solution 3.1.4. We start by solving Eq. (3.18) to find

$$B_j(s) = \frac{\lambda_j^*}{i\hbar s - \epsilon_j}. \tag{3.20}$$

We then substitute this into Eq. (3.17) to find

$$(i\hbar s - \epsilon_0)A(s) - \sum_j \frac{|\lambda_j|^2}{i\hbar s - \epsilon_j} A(s) = i\hbar, \tag{3.21}$$

which is of the desired form with

$$\Sigma(is) = \sum_j \frac{|\lambda_j|^2}{i\hbar s - \epsilon_j}. \tag{3.22}$$

3.1.5. In the thermodynamic limit, the leads should contain a dense set of modes. Hence it is desirable to replace the sums with integrals. We define a "spectral density",

$$S(\omega) = \sum_j |\lambda_j|^2 2\pi\delta(\hbar\omega - \epsilon_j). \tag{3.23}$$

Show that

$$\Sigma(is) = \int \frac{d\hbar\omega}{2\pi} \frac{S(\omega)}{i\hbar s - \hbar\omega}. \tag{3.24}$$

Solution 3.1.5. The result comes from a simple substitution.

3.1.6. The simplest model for $S(\omega)$ is that is is a constant: $S(\omega) = S$. Assuming that the real part of s is positive, show that $\Sigma(is) = -i\hbar\Gamma/2$. Find Γ.

Solution 3.1.6. The integral is over an infinite domain, which is most easily considered by introducing a cutoff Ω and taking $\Omega \to \infty$,

$$\begin{aligned}
\Sigma(is) &= S\int_{-\hbar\Omega}^{\hbar} \Omega \frac{d\hbar\omega}{2\pi} \frac{1}{i\hbar s - \hbar\omega} && (3.25)\\
&= -\frac{S}{2\pi} \log\left(\frac{i\hbar s - \hbar\Omega}{i\hbar s + \hbar\Omega}\right) && (3.26)\\
&= \frac{-iS}{2}. && (3.27)
\end{aligned}$$

Thus $\Gamma = S/\hbar$.

3.1.7. We thus arrive at

$$A(s) = \frac{i\hbar}{i\hbar s - (\epsilon - i\hbar\Gamma/2)}. \tag{3.28}$$

Invert the Laplace transform to find $A(t)$.

Solution 3.1.7. We know that

$$\int dt e^{-st} e^{-iEt/\hbar} = \frac{1}{s + iE/\hbar} = \frac{i\hbar}{i\hbar s - E}. \tag{3.29}$$

We further know

$$\int dt e^{-st} A(t) = \frac{i\hbar}{i\hbar s - (\epsilon - i\hbar\Gamma/2)}. \tag{3.30}$$

Thus

$$A(t) = e^{-i(\epsilon - i\hbar\Gamma/2)t/\hbar} = e^{-\Gamma t/2} e^{-i\epsilon t/\hbar}. \tag{3.31}$$

3.1.8. What is the probability that the particle is on the dot at time t?

Solution 3.1.8.

$$P(t) = |A(t)|^2 = e^{-\Gamma t}. \tag{3.32}$$

A.1. Discussion

The calculation we just did should feels somewhat satisfying, and the main punch-line is that the occupation of the cavity mode decays exponentially. The decay rate is proportional to the product of the square of the coupling to the environment, and the density of states.

There are a couple aspects which might seem less than ideal. In particular, choice for the spectral density may have felt arbitrary, and as presented it was not clear how valid/generic our approximations were. What does this "self-energy" mean?

Over the next few classes we will answer these questions.

B. Greens functions

As you know from your mathematics courses, a Greens function is the solution to an inhomogeneous differential equation where the inhomogeneous term is a delta-function. It turns out that we can interpret the $A(t)$ from section A as a Greens function – at least if we appropriately specify its behavior for $t < 0$. That is, we define

$$G^R_{aa}(t) = \frac{1}{i\hbar}\theta(t)A(t) \tag{3.33}$$

where $\theta(t)$ is the Heaviside step function, which vanishes for $t < 0$ and is unity for $t > 0$. The R denotes the fact that it is a "Retarded" Greens function, which vanishes when $t < 0$. The aa denotes the fact that it gives the amplitude of being in the a mode, given that one starts at $t = 0$ in the a mode. By the same logic, we can write

$$G^R_{aj}(t) = \frac{1}{i\hbar}\theta(t)B_j(t) \tag{3.34}$$

as the amplitude to end up in state j at time t, assuming that you start on the dot. To save ink, I will leave off the R.

As the notation suggests, one can also write functions G_{ja} and G_{jk} which represent amplitude of ending up in state a or k, assuming at time $t = 0$ you are in state j.

From the equations of motion for $A(t)$ and $B_j(t)$,

$$i\hbar\partial_t G_{aa}(t) - \epsilon_0 G_{aa}(t) - \sum_j \lambda_j G_{aj}(t) = \delta(t) \tag{3.35}$$

$$i\hbar\partial_t G_{aj}(t) - \epsilon_j G_{aj}(t) - \lambda^*_j G_{aa}(t) = 0. \tag{3.36}$$

Indeed we see that G_{aa} is a Greens function.

Problem 3.2.

3.2.1. Fourier transform these equations to show that

$$G_{aa}(\omega) = \frac{1}{\omega - \epsilon_0 - \Sigma(\omega)}. \tag{3.37}$$

Solution 3.2.1. The argument is the same as that we made for A. Explicitly,

$$\hbar\omega G_{aa} - \epsilon_0 G_{aa} - \sum_j \lambda_j G_{aj} = 1 \tag{3.38}$$

$$\hbar\omega G_{aj} - \epsilon_j G_{aj} - \lambda^*_j G_{aa} = 0.. \tag{3.39}$$

We then solve the second equation for G_{aj} to find

$$G_{aj} = \frac{\lambda_j}{\hbar\omega - \epsilon_j} G_{aa}. \tag{3.40}$$

Substituting this back into the first equation yields

$$\left(\hbar\omega - \epsilon_0 - \sum_j \frac{|\lambda_j|^2}{\hbar\omega - \epsilon_j}\right) G_{aa} = 1, \tag{3.41}$$

which is the desired expression.

C. Eigenstates

A complementary way to solve this decay problem is to find all the eigenstates of the system+bath, and then expand the initial wavefunction in terms of these states. Here we will learn how to find these states. It will be a gentle introduction to a bit more machinery.

Suppose we know all the eigenstates $|\alpha\rangle$ and their energy E_α. The generic eigenstate will be of the form

$$|\alpha\rangle = A^\alpha \hat{a}^\dagger|\text{vac}\rangle + \sum_j B_j^\alpha \hat{b}_j^\dagger|\text{vac}\rangle. \tag{3.42}$$

These coefficients are clearly

$$A^\alpha = \langle a|\alpha\rangle \tag{3.43}$$
$$B_j^\alpha = \langle a|j\rangle, \tag{3.44}$$

where

$$|a\rangle = a^\dagger|\text{vac}\rangle \tag{3.45}$$
$$|j\rangle = b_j^\dagger|\text{vac}\rangle. \tag{3.46}$$

At time $t = 0$ we are in the state

$$|a\rangle = \sum_\alpha \langle\alpha|a\rangle|\alpha\rangle \tag{3.47}$$
$$= \sum_\alpha (A^\alpha)^*|\alpha\rangle. \tag{3.48}$$

Thus

$$|t\rangle = \sum_\alpha (A^\alpha)^* e^{-iE_\alpha t}|\alpha\rangle. \tag{3.49}$$

The amplitude of being on the dot at time t is

$$A(t) = \langle a|t\rangle = \sum_\alpha (A^\alpha)^* e^{-iE_\alpha t}\langle a|\alpha\rangle \tag{3.50}$$
$$= \sum_\alpha |A^\alpha|^2 e^{-iE_\alpha t}. \tag{3.51}$$

Problem 3.3. Eigenstates

3.3.1. Use the time-independent Schrodinger's equation

$$\hat{H}|\alpha\rangle = E_\alpha|\alpha\rangle \tag{3.52}$$

to find an equation satisfied by the coefficients A^α and B_j^α. Note: this may feel repetitive. That is intentional, you should start to get a feel for the fact that these various problems: time evolving an initial state, finding the Greens function for the Schrodinger equation, and finding eigenstates, are all intimately related.

Solution 3.3.1.

$$\hat{H}|\alpha\rangle = A^\alpha \hat{H}\hat{a}^\dagger|\text{vac}\rangle + \sum_j B_j^\alpha \hat{H}\hat{b}_j^\dagger|\text{vac}\rangle \tag{3.53}$$

$$= \left[A^\alpha(\epsilon_0 a^\dagger + \sum_j \lambda_j^* \hat{b}_j^\dagger) + \sum_j B_j^\alpha(\epsilon_j b_j^\dagger + \lambda_j \hat{a})\right]|\text{vac}\rangle \tag{3.54}$$

$$= \left[\epsilon_0 A^\alpha + \sum_j \lambda_j B_j^\alpha\right]\hat{a}^\dagger|\text{vac}\rangle + \sum_j \left[\epsilon_j B_j^\alpha + A^\alpha \lambda_j^*\right]\hat{b}_j^\dagger|\text{vac}\rangle \tag{3.55}$$

but this should equal

$$E_\alpha|\alpha\rangle = E_\alpha A^\alpha|\text{vac}\rangle + \sum_j E_\alpha B_j^\alpha b_j^\dagger|\text{vac}\rangle. \tag{3.56}$$

Equating coefficients gives

$$\epsilon_0 A^\alpha + \sum_j \lambda_j B_j^\alpha = E_\alpha A^\alpha \tag{3.57}$$

$$\epsilon_j B_j^\alpha + A^\alpha \lambda_j^* = E_\alpha B_j. \tag{3.58}$$

3.3.2. Show that B_j^α can be eliminated to give

$$(\epsilon_0 - \Sigma(E_\alpha))\, A^\alpha = E_\alpha A^\alpha. \tag{3.59}$$

Solution 3.3.2. This should be old hat by now. We write

$$B_j^\alpha = -\frac{\lambda_j^*}{E_\alpha - \epsilon_j} A^\alpha, \tag{3.60}$$

which gives

$$\left(\epsilon_0 - \sum_j \frac{|\lambda_j|^2}{E_\alpha - \epsilon_j}\right) A^\alpha = E_\alpha A^\alpha, \tag{3.61}$$

which is the desired equation.

C.1. Discussion

Here we see an excellent interpretation of the self-energy. It is the contribution to the system Hamiltonian which you get from integrating out the environment. IE. We interpret

$$\hat{H}_{\text{eff}} = (\epsilon_0 - \Sigma(E))\hat{a}^\dagger \hat{a} \tag{3.62}$$

as an effective Hamiltonian.

D. Homework: Due Feb 2

Problem 3.4. Fermi's Golden Rule Here we will perturbative solve the equations of motion for this decaying system:

$$i\hbar A'(t) = \epsilon_0 A(t) + \sum_j \lambda_j B_j(t) \tag{3.63}$$

$$i\hbar B_j'(t) = \epsilon_j B_j(t) + \lambda_j^* A(t), \tag{3.64}$$

with boundary conditions $A(0) = 1$ and $B_j(0) = 0$. We will formally treat λ_j as a small parameter.

This is an argument that you should have seen in your quantum mechanics class, where it is known as "Fermi's Golden Rule." It is one of those things that you usually concentrate on the result rather than the derivation.

3.4.1. First, if $\lambda_j = 0$ find $A(t)$ and $B_j(t)$. These will be the zeroth order solutions $A^0(t)$ and $B_j^0(t)$.

Solution 3.4.1. The equations decouple. The B equations are simple, one just has

$$B_j^0(t) = 0. \tag{3.65}$$

The A equation yields

$$A^0(t) = e^{-i\epsilon_0 t/\hbar}. \tag{3.66}$$

3.4.2. On the right hand side of Eq. (3.64), replace $A(t)$ with $A^0(t)$ to get an inhomogeneous differential equation of the form

$$[i\hbar\partial_t - \epsilon_j]\, B_j(t) = c_j e^{-i\epsilon_0 t/\hbar}. \tag{3.67}$$

What is the constant c_j? Integrate this differential equation. Call the solution $B_j^1(t)$.

Solution 3.4.2. Making the substitution, we get

$$\left[i\hbar\partial_t - \epsilon_j\right] B_j(t) = \lambda_j^* e^{-i\epsilon_0 t/\hbar}, \tag{3.68}$$

so $c_j = \lambda_j^*$. There are at least 3 ways to solve this equations: Integrating factors, Greens functions, and Guessing. We use integrating factor, noting that

$$e^{i\epsilon_j t/\hbar}\left(i\hbar\partial_t\right)\left(e^{-i\epsilon_j t/\hbar}B_j(t)\right) = \left[i\hbar\partial_t - \epsilon_j\right] B_j(t). \tag{3.69}$$

Thus our equation becomes

$$\left(i\hbar\partial_t\right)\left(e^{-i\epsilon_j t/\hbar}B_j(t)\right) = \lambda_j^* e^{-i(\epsilon_0-\epsilon_j)t/\hbar}, \tag{3.70}$$

which gives

$$e^{i\epsilon_j t/\hbar}B_j(t) = \frac{\lambda_j^*}{\epsilon_0 - \epsilon_t}\left[e^{-i(\epsilon_0-\epsilon_j)t/\hbar} - 1\right], \tag{3.71}$$

or

$$B_j(t) = \frac{\lambda_j^*}{\epsilon_0 - \epsilon_j}\left[e^{-i\epsilon_0 t/\hbar} - e^{-i\epsilon_j t/\hbar}\right]. \tag{3.72}$$

3.4.3. On the right hand side of Eq. (3.63), replace $B(t)$ with $B^1(t)$ to get an inhomogeneous differential equation of the form

$$\left[i\hbar\partial_t - \epsilon_0\right] A(t) = \sum_j \left[u_j e^{-i\epsilon_j t} - v_j e^{-i\epsilon_0 t}\right]. \tag{3.73}$$

Find u_j and v_j. Do not integrate the equation.

Solution 3.4.3. Making the substitution we find

$$\left[i\hbar\partial_t - \epsilon_0\right] A(t) = \sum_j \frac{|\lambda_j|^2}{\epsilon_0 - \epsilon_j}\left[e^{-i\epsilon_j t/\hbar} - e^{-i\epsilon_0 t/\hbar}\right], \tag{3.74}$$

from which we conclude

$$u_j \quad = \quad v_j = \frac{|\lambda_j|^2}{\epsilon_0 - \epsilon_j}. \tag{3.75}$$

3.4.4. So far everything has been straightforward. We now get to the hard part of the argument. Your results from the last question should be equivalent to

$$i\hbar\partial_t\left[e^{i\epsilon_0 t/\hbar}A(t)\right] = \int \frac{d\omega}{2\pi}\Gamma(\omega)\frac{e^{-i(\epsilon_0-\omega)t/\hbar} - 1}{\epsilon_0 - \omega}. \tag{3.76}$$

where

$$\Gamma(\omega) = \sum_j |\lambda_j|^2 2\pi\delta(\omega - \epsilon_j). \tag{3.77}$$

Verify that this expression is correct.

Solution 3.4.4. We start by evaluating the derivative, and using our previous result to write.

$$\begin{aligned} i\hbar\partial_t \left[e^{i\epsilon_0 t/\hbar}A(t)\right] &= e^{i\epsilon_0 t}\left[i\hbar\partial_t A(t) - \epsilon_0 A(t)\right] && (3.78)\\ &= e^{i\epsilon_0 t}\sum_j \frac{|\lambda_j|^2}{\epsilon_0-\epsilon_j}\left[e^{-i\epsilon_j t/\hbar} - e^{-i\epsilon_0 t/\hbar}\right] && (3.79)\\ &= \sum_j \frac{|\lambda_j|^2}{\epsilon_0-\epsilon_j}\left[e^{i(\epsilon_0-\epsilon_j)t/\hbar} - 1\right]. && (3.80)\end{aligned}$$

We then introduce an integral over ω and a delta function to get

$$i\hbar\partial_t \left[e^{i\epsilon_0 t/\hbar}A(t)\right] = \int \frac{d\omega}{2\pi}\sum_j 2\pi\delta(\omega-\epsilon_j)\frac{|\lambda_j|^2}{\epsilon_0-\omega}\left[e^{-i\omega t/\hbar} - e^{-i\epsilon_0 t/\hbar}\right]. \quad (3.81)$$

Reversing the order of the sum and integral gives the desired expression.

3.4.5. The function $\frac{e^{-i(\epsilon_0-\omega)t/\hbar}-1}{\epsilon_0-\omega}$ is a strongly peaked function of ω, with height proportional to t, and width proportional to $1/t$. Thus in the limit $t\to 0$ it acts like a delta-function. In particular, if we assume $\Gamma(\omega)$ is smooth on the scale of this term, we can approximate

$$i\hbar\partial_t \left[e^{i\epsilon_0 t/\hbar}A(t)\right] \approx \Gamma(\epsilon_0)\int \frac{d\omega}{2\pi}\frac{e^{-i(\epsilon_0-\omega)t/\hbar}-1}{\epsilon_0-\omega}. \quad (3.82)$$

This integral can be calculated in closed form. Find its value. This completes the derivation of "Fermi's Golden Rule."

Solution 3.4.5. The real part of the integral is odd about $\omega=\epsilon_0$, so only the inaginary part is non-zero, thus

$$\begin{aligned}\int \frac{d\omega}{2\pi}\frac{e^{-i(\epsilon_0-\omega)t/\hbar}-1}{\epsilon_0-\omega} &= -i\int\frac{dx}{2\pi}\frac{\sin(x)}{x} && (3.83)\\ &= -i/2, && (3.84)\end{aligned}$$

where the last is a tabulated integral. There are may different ways to do the integral – look up "Dirichlet integral" on Wikipedia for 4 of them.

3.4.6. In class we argued that

$$A(t) = e^{-i(\epsilon - i\hbar\Gamma/2)t/\hbar} = e^{-\Gamma t/2}e^{-i\epsilon t/\hbar}. \quad (3.85)$$

where, for the case of frequency-independent self-energy

$$\Gamma = \frac{2}{\hbar}\mathrm{Im}\Sigma, \quad (3.86)$$

with

$$\Sigma(\omega) = \sum_j \frac{|\lambda_j|^2}{\hbar\omega - \epsilon_j}. \tag{3.87}$$

Use the expression

$$\frac{1}{x} = \frac{P}{x} \pm i\pi\delta(x) \tag{3.88}$$

to calculate Γ. How does it compare to the Fermi's Golden Rule result?

Problem 3.5. Non-uniform self-energy In the lecture we assumed that Σ was independent of ω. In the generic case, behavior of $G^R(t)$ will essentially be given by the result we used, where you just evaluate $\Sigma(\omega)$ at some particular frequency.

3.5.1. Start with

$$G^R(t) = \int \frac{d\omega}{2\pi} \frac{e^{-i\omega t}}{\omega - \epsilon_0 - \Sigma(\omega)}, \tag{3.89}$$

Suppose we can Taylor expand Σ about $\omega = \epsilon_0$,

$$\Sigma(\omega) = (\delta + i\Gamma/2) + \frac{(\omega - \epsilon_0)}{D}(u + iv) + \mathcal{O}(D^{-2}), \tag{3.90}$$

where δ, Γ, u, v should all be of similar magnitude, and D is a large energy corresponding to the scale on which Σ changes. It is of order the band-width. The neglected terms are smaller in the bandwidth. Calculate $G(t)$ both with and without the $1/D$ term. You should find that the corrections are small – lending credulence to the leading order approximation.

Chapter 4

Greens functions in finite Hilbert spaces – Feb 2, 2018

Last day we motivated the idea that we could understand the dynamics of open systems by calculating Greens functions. Today we will further understand these mathematical objects in the context of isolated finite systems. We will work with tight-binding models, but all of our arguments also apply to the continuum – they are just slightly more abstract there, and the linear algebra turns into differential equations.

This lecture is in part making you feel more comfortable with the tools. Next week we will show how to use the Greens functions to calculate transport.

A. Tight-Binding Models

Tight binding models play an important role in solid-state physics. They are used to build-up the physics of a material or device, starting with atomic orbitals. Alternatively (as discussed in section B) they are a systematic way to truncate the infinite Hilbert space of a continuum system, in order to either get insight or simplify calculations.

I assume you are familiar with the idea of tight-binding models. The simplest example is a double-well. You know that the low energy physics of a double-well can be approximated by simply taking two states: one that lies on the left well, and one on the right. A tight-binding model is simply the generalization of this to multiple wells. One may take multiple states on each well – these are referred to as orbitals.

Given N_s sites, each with n_0 orbitals, the single-particle Hamiltonian can be written as a $N_s \times n_0$ by $N_s \times n_0$ matrix. The terms which connect orbitals on

different sites are referred to as "hopping matrix elements". Typically the size of the hopping matrix elements fall off exponentially with the spacing between sites, and we truncate to just a few.

For example, consider a 1D chain with one orbital per site. We let $\hat{a}_j$ be the operator which removes a particle from site j. A typical tight-binding model with nearest neighbor hopping might be

$$\hat{H} = -J \sum_j \left(\hat{a}^\dagger_{j+1} \hat{a}_j + \hat{a}^\dagger_j \hat{a}_{j+1} \right). \tag{4.1}$$

A generic tight-binding model is

$$\hat{H} = \sum_{ij} H_{ij} \hat{a}^\dagger_i \hat{a}_j, \tag{4.2}$$

where H_{ij} are just numbers corresponding to matrix elements of the Hamiltonian,

$$H_{ij} = \langle i | \hat{H} | j \rangle, \tag{4.3}$$

where $|j\rangle = a^\dagger_j |\text{vac}\rangle$ is the state where a particle is on site j.

A.1. Statistics

Most of the physics in this course is single-particle physics, and we are really just using the creation and annihilation operators for the notational ease they provide. It is, however, worth remembering that their true utility is in helping keep track of the symmetries of many-particle wavefunctions. In particular the symmetry is encoded in commutation/anticommutation relations

$$[a_i, a^\dagger_j] = a_i a^\dagger_j - a^\dagger_j a_i = \delta_{ij} \qquad \text{(Bose)} \tag{4.4}$$

$$[a_i, a^\dagger_j] = a_i a_j - a_j a_i = 0 \qquad \text{(Bose)} \tag{4.5}$$

$$\{a_i, a^\dagger_j\} = a_i a^\dagger_j + a^\dagger_j a_i = \delta_{ij} \qquad \text{(Fermi)} \tag{4.6}$$

$$\{a_i, a^\dagger_j\} = a_i a_j + a_j a_i = 0. \qquad \text{(Fermi).} \tag{4.7}$$

If these are unfamiliar to you, let me know and I will give you some reading – there is one homework problem from today that uses them, and about 5 minutes of today's lecture.

A.2. Schrodinger Picture

The single-particle Schrodinger equation for a tight-binding model is just a matrix equation.

Problem 4.1.

4.1.1. Take $|\psi\rangle = \sum_j \psi_j |j\rangle$. If this is an eigenstate of the Hamiltonian, $\hat{H}|\psi\rangle = E|\psi\rangle$, find an equation obeyed by the coefficients ψ_j.

These sorts of matrix equations are trivial to solve numerically. Your laptop should be able to essentially instantaneously diagonalize matrices which are $10,000 \times 10,000$.

A.3. Heisenberg Picture

It will be convenient to also be able to operate in the Heisenberg picture – where one thinks about the properties of operators instead of states. In particular consider the case in which we have a tight-binding model with N states. We will find it useful to understand transformations of the form

$$\hat{b}_s = \sum_j U_{sj} \hat{a}_j, \tag{4.8}$$

where U is a $N \times N$ matrix. That is, we have defined operators $\hat{b}_s$ which involve removing particles from a superposition of states. The concrete example we are thinking of, is that we want the b_s's to correspond to the eigenstates of the single particle Hamiltonian.

Suppose we have fermions: that is $\{a_i, a_j^\dagger\} = \delta_{ij}$ and $\{a_i, a_j\} = 0$. We call the transformation in Eq. (4.8) canonical if $\{b_s, b_t^\dagger\} = \delta_{st}$ and $\{b_s, b_t\} = 0$. For Bose operators we use commutators instead of anticommutators.

Physically, a canonical transformation means that the new operators describe independent modes: adding or removing a particle from one mode does not affect other modes. It also means that they are properly "normalized".

Problem 4.2.

4.2.1. Show that Eq. (4.8) is canonical if and only if U is unitary: $U^\dagger U = 1$.

One consequence is that

$$\hat{a}_j = \sum_s (U^{-1})_{js} \hat{b}_s \tag{4.9}$$

$$= \sum_s (U^\dagger)_{js} \hat{b}_s \tag{4.10}$$

$$= \sum_s U^*_{sj} \hat{b}_s \tag{4.11}$$

We can always choose U to diagonalize H_{ij}, that is we can always find a unitary matrix such that

$$(UHU^\dagger)_{st} = \delta_{st} \epsilon_s. \tag{4.12}$$

In that case

$$\hat{H} = \sum_{ij} \hat{a}_i^\dagger H_{ij} \hat{a}_j \tag{4.13}$$

$$= \sum_{st} \hat{b}_s^\dagger \left(UHU^\dagger\right)_{st} \hat{b}_t \tag{4.14}$$

$$= \sum_s \epsilon_s \hat{b}_s^\dagger \hat{b}_s. \tag{4.15}$$

B. Tight-Binding Models as Finite Difference Approximations to Continuum Systems

A second, important application of tight-binding models is as approximations to continuum systems. We will limit ourselves to a simple example. Consider the Schrodinger equation:

$$-\frac{\hbar^2}{2m}\partial_x^2\psi(x) + V(x)\psi(x) = E\psi(x). \tag{4.16}$$

We can approximate the derivative by considering the Taylor expansion

$$\psi(x+\delta) = \psi(x) + \delta\psi'(x) + \frac{\delta^2}{2}\psi''(x) + \cdots \tag{4.17}$$

$$\psi(x-\delta) = \psi(x) - \delta\psi'(x) + \frac{\delta^2}{2}\psi''(x) + \cdots \tag{4.18}$$

which motivates

$$\partial_x^2\psi(x) \approx \frac{\psi(x+\delta) + \psi(x-\delta) - 2\psi(x)}{\delta^2}. \tag{4.19}$$

If we define $\psi_j = \psi(j\delta)$, and $V_j = V(j\delta)$ then Eq. (4.16) becomes

$$-J(\psi_{j+1} + \psi_{j-1}) + (V_j + 2J)\psi_j = E\psi_j, \tag{4.20}$$

where $J = \hbar^2/(2m\delta^2)$. Well this is the exact same Schrodinger equation as we would get from the tight-binding model

$$\hat{H} = \sum_j -J(\hat{a}_{j+1}^\dagger \hat{a}_j + \hat{a}_j^\dagger \hat{a}_{j+1}) + (V_j + 2J)\hat{a}_j^\dagger \hat{a}_j. \tag{4.21}$$

C. Time dependent Schrodinger Equation

The time-dependent Schrodinger Equation is also a matrix equation. We write $|\psi\rangle = \sum_j \psi_j(t)|j\rangle$, and consider

$$i\hbar\partial_t|\psi\rangle = \hat{H}|\psi\rangle, \tag{4.22}$$

which gives

$$i\hbar\partial_t\psi_i(t) = \sum_i H_{ij}\psi_j(t). \tag{4.23}$$

Given an initial value $\psi(t=0)$, we can solve the time-dependent Schrodinger equation using the Greens function

$$\psi_i(t) = \sum_j G^R_{ij}(t)\psi_j(0), \tag{4.24}$$

where

$$i\hbar\partial_t G^R_{ij}(t) - \sum_k H_{ik}G^R_{kj}(t) = \delta(t)\delta_{ij} \tag{4.25}$$

with $G^R_{ij}(t<0) = 0$. The Fourier transform of the Greens function is particularly simple,

$$\sum_k (\hbar\omega\delta_{ik} - H_{ik})G_{kj}(\omega) = \delta_{ij}. \tag{4.26}$$

This is nothing but the matrix equation

$$G(\omega) = \frac{1}{\omega - H}. \tag{4.27}$$

If you have H represented as a big matrix, one just needs to do matrix inversion to calculate G.

Note: Eq. (4.27) is somewhat ambiguous, since the matrix $\omega - H$ is not invertible whenever ω is equal to one of the eigenvalues of H. This ambiguity exactly corresponds to the fact that the Greens functions are not unique: you need to specify boundary conditions. As you will see in the homework, an unambiguous Fourier transform of the retarded Greens function is

$$G(\omega) = \lim_{\eta\to 0^+} \frac{1}{\omega - H - i\eta}. \tag{4.28}$$

Since the eigenstate of H are all real, the matrix $\omega - H - i\eta$ is invertible for any $\eta \neq 0$. For most of these notes I won't bother with adding this infinitesmal. We can always put it in when we encounter any ambiguities.

D. What can you do with $G(\omega)$

I think it is pretty clear what one can do with $G(t)$: You can time-evolve a wavefunction: $G^R_{ij}(t)$ is the amplitude that if you start at site j at time 0, you end up at site i at time t.

It turns out that there are a number of very useful things that one can do directly with the Fourier transform, $G(\omega)$.

D.1. Response to a perturbation

First of all, like any other Greens function, $G(\omega)$ tells you about the response of the system to an external perturbation of frequency ω. That is if

$$i\hbar\partial_t\psi - H\psi = \psi_0 e^{-i\nu t}, \tag{4.29}$$

then once the transients die down,

$$\psi_i = e^{-i\nu t}\sum_j G_{ij}(\nu)(\psi_0)_j. \tag{4.30}$$

This will clearly be a useful result when we are trying to calculate currents from leads: The leads will act like external perturbations, and the Greens function will allow us to calculate how these disturbances propagate.

D.2. Spectral Representation

It turns out that there are other useful things that we can extract from G. These are most transparent in the *Spectral Representation*. Let ψ_j^s be the s'th eigenstate of H_{ij}. By Construction

$$H_{ij} = \sum_s (\psi_i^s)^* E_s \psi_i^s. \tag{4.31}$$

Equivalently

$$\hat{H} = \sum_s |s\rangle E_s \langle s|. \tag{4.32}$$

Clearly the Greens function is then

$$\hat{G}(\omega) = \frac{1}{\omega - \hat{H}} = \sum_s |s\rangle \frac{1}{\omega - E_s}\langle s| \tag{4.33}$$

or

$$G_{ij}(\omega) = \sum_s \frac{(\psi_i^s)^*\psi_j^s}{\omega - E_s}. \tag{4.34}$$

Thus one can find eigenstates by looking at the poles of G.

Mathematically, we can more directly access this information by using the identity that

$$\frac{1}{x \pm i\eta} = \frac{P}{x} \mp i\pi\delta(x), \tag{4.35}$$

where P represents the principle part.

This relation is usually proven by noting that for any function $f(x)$ one can write

$$\begin{aligned} I &= \lim_{\eta\to 0}\int_{-\infty}^{\infty} dx\, \frac{f(x)}{x \pm i\eta} && (4.36)\\ &= \lim_{\epsilon\to 0}\lim_{\eta\to 0}\left(\int_{-\infty}^{-\epsilon} + \int_{\epsilon}^{\infty}\right)\frac{f(x)}{x\pm i\eta} && (4.37)\\ &\quad + \lim_{\epsilon\to 0}\lim_{\eta\to 0}\int_{-\epsilon}^{\epsilon}\frac{f(x)}{x\pm i\eta}. \end{aligned}$$

The first integral is well behaved as $\eta \to 0$, and we define

$$\int_{-\infty}^{\infty} f(x)\frac{P}{x} = \lim_{\epsilon\to 0}\left(\int_{-\infty}^{-\epsilon} + \int_{eps}^{\infty}\right)\frac{f(x)}{x}. \quad (4.38)$$

The second integral is over a small range of x, and we write

$$\begin{aligned} \lim_{\epsilon\to 0}\lim_{\eta\to 0}\int_{-\epsilon}^{\epsilon}\frac{f(x)}{x\pm i\eta} &= f(0)\lim_{\epsilon\to 0}\lim_{\eta\to 0}\int_{-\epsilon}^{\epsilon}\frac{1}{x\pm i\eta} && (4.39)\\ &= f(0)\lim_{\epsilon\to 0}\lim_{\eta\to 0}\log\left(\frac{\epsilon\pm i\eta}{-\epsilon\pm i\eta}\right) && (4.40)\\ &= \mp i\pi f(0). && (4.41) \end{aligned}$$

Regardless, we can use the Greens function to calculate the spectral function

$$\begin{aligned} A_{ij}(\omega) &= \sum_s (\psi_i^s)^* \psi_j^s 2\pi\delta(\omega - E_s) && (4.42)\\ &= 2\,\mathrm{Im}G(\omega - i\eta) && (4.43)\\ &= 2\,\mathrm{Im}G^R(\omega) && (4.44) \end{aligned}$$

In particular, we can access the density of states as

$$\begin{aligned} \rho(\omega) &= \sum_s 2\pi\delta(\omega - E_s) && (4.45)\\ &= \mathrm{Tr}A(\omega). && (4.46) \end{aligned}$$

D.3. Calculating Transport

Both the Greens function and the spectral function will be a key part of our transport calculations.

E. Homework: Due Feb 9

Problem 4.3. Greens function for 2-level system Suppose we have a 2-level system with Hamiltonian

$$H = \begin{pmatrix} 0 & -J \\ -J & 0 \end{pmatrix}. \quad (4.47)$$

4.3.1. Calculate the 2×2 matrix $G^R(\omega)$.

Solution 4.3.1.

$$G^R(\omega) = \begin{pmatrix} \omega & J \\ J & \omega \end{pmatrix}^{-1} \tag{4.48}$$

$$= \frac{1}{\omega^2 - J^2} \begin{pmatrix} \omega & -J \\ -J & \omega \end{pmatrix} \tag{4.49}$$

4.3.2. Calculate the 2×2 matrix $G^R(t)$.

Solution 4.3.2. There are a number of ways to calculate this, for example we can find the eigenvalues and eigenvectors of H:

$$\psi_1 = \begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix} \quad E_1 = -J \tag{4.50}$$

$$\psi_2 = \begin{pmatrix} 1/\sqrt{2} \\ -1/\sqrt{2} \end{pmatrix} \quad E_2 = J \tag{4.51}$$

then

$$G^R(t) = \frac{1}{i}\theta(t)e^{-iE_1 t}\psi_1\psi_1^\dagger + \frac{1}{i}\theta(t)e^{-iE_2 t}\psi_2\psi_2^\dagger \tag{4.52}$$

$$= \frac{1}{2i}\theta(t)e^{iJt}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} + \frac{1}{2i}\theta(t)e^{-iJt}\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} \tag{4.53}$$

$$= \frac{1}{i}\theta(t)\begin{pmatrix} \cos(Jt) & i\sin(Jt) \\ i\sin(Jt) & \cos(Jt) \end{pmatrix}. \tag{4.54}$$

An alternative approach is to note that

$$\mathbf{H}^2 = J^2\mathbf{I} \tag{4.55}$$

where $\mathbf{I}$ is the 2×2 identity matrix. Then

$$G^R(t) = \frac{1}{i}\theta(t)e^{-iHt} \tag{4.56}$$

$$= \frac{1}{i}\theta(t)\left[\cos(Ht)\mathbf{I} - i\mathbf{H}t\frac{\sin(Ht)}{Ht}\right] \tag{4.57}$$

$$= \frac{1}{i}\theta(t)\left[\cos(Jt)\mathbf{I} - i\mathbf{H}t\frac{\sin(Jt)}{Jt}\right], \tag{4.58}$$

which is readily seen to agree with the previous argument.

4.3.3. Calculate the 2×2 matrix $A(t)$.

Solution 4.3.3.

$$A(t) = \begin{pmatrix} \cos(Jt) & i\sin(Jt) \\ i\sin(Jt) & \cos(Jt) \end{pmatrix}. \tag{4.59}$$

Problem 4.4. Branch cuts and Greens Functions

This problem works you through all the details about the infinitesmal imaginary bits.

4.4.1. There was a typo in this question – the correct expression is in red

Consider

$$G^R(t) = e^{-i(\epsilon - i\eta)t}\frac{1}{i}\theta(t). \tag{4.60}$$

Show that as $\eta \to 0^+$, this function obeys

$$(i\partial_t - \epsilon)G^R(t) = \delta(t). \tag{4.61}$$

Solution 4.4.1.

$$i\partial_t G^R(t) = (\epsilon - i\eta)e^{-i(\epsilon - i\eta)t}\frac{1}{i}\theta(t) + e^{-i(\epsilon - i\eta)t}\delta(t), \tag{4.62}$$

where we have used that the derivative of the step function is a delta-function. We then use $f(t)\delta(t) = f(0)\delta(t)$ and take the limit $\eta \to 0$ to find

$$i\partial_t G^R(t) = \epsilon G^R(t) + \delta(t) \tag{4.63}$$

which is the desired result.

4.4.2. Calculate the Fourier transform

$$G^R(\omega) = \int dt e^{i\omega t} G^R(t). \tag{4.64}$$

What is the condition on η for the integral to be absolutely convergent?

Solution 4.4.2. If $\eta > 0$, then the integral is convergent and equal to

$$G^R(\omega) = \frac{1}{\omega - \epsilon + i\eta}. \tag{4.65}$$

4.4.3. There was a typo in this question – the correct expression is in red

Consider

$$G^A(t) = e^{-i(\epsilon + i\eta)t}\frac{-1}{i}\theta(-t). \tag{4.66}$$

Show that as $\eta \to 0^+$, this function obeys

$$(i\partial_t - \epsilon)G^A(t) = \delta(t). \tag{4.67}$$

Solution 4.4.3.

$$i\partial_t G^A(t) = (\epsilon + i\eta)e^{-i(\epsilon+i\eta)t}\frac{-1}{i}\theta(-t) + e^{-i(\epsilon+i\eta)t}\delta(t) \tag{4.68}$$

Again taking the limit $\eta \to 0$ gives the desired equation.

4.4.4. Calculate the Fourier transform

$$G^A(\omega) = \int dt e^{i\omega t} G^A(t). \tag{4.69}$$

What is the condition on η for the integral to be absolutely convergent?

Solution 4.4.4. Again the integral is convergent if $\eta > 0$ in which case

$$G^A(\omega) = \frac{1}{\omega - \epsilon - i\eta} \tag{4.70}$$

4.4.5. Use contour integrals to calculate

$$f(t) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{e^{-i\omega t}}{\omega - \epsilon - i\eta} \tag{4.71}$$

for $\eta > 0$.

If you have never done this integral before, the way to do it is to separately consider the case $t > 0$ and $t < 0$. If $t > 0$ then the integrand vanishes when the imaginary part of ω becomes large and negative. Thus you can replace the integral with a contour integral which consists of the real axis, and an arc which extends through the lower-half plane. On the other hand, when $t < 0$, the integrand becomes small when ω is large and positive – in which case you can close the contour in the upper-half plane.

Solution 4.4.5. Following the hint, for $t > 0$ the contour includes no poles, and thus $f(t) = 0$ for $t > 0$, Conversely if $t < 0$ there is a pole at $\omega = \epsilon + i\eta$ which gives

$$f(t) = \frac{-1}{i}\theta(-t)e^{-i(\epsilon+i\eta)t}. \tag{4.72}$$

Problem 4.5. Greens functions from operator equations of motion This course is all about Greens functions in the case where we can neglect the electron-electron interactions. It is useful, however, to know how to generalize them to the interacting many-body problem. This generalization will also provide us with some notation that we will use in future lectures.

In that case one simply defines

$$G^R_{ij}(t,t') = \frac{1}{i\hbar}\theta(t-t')\langle \hat{a}_i(t)\hat{a}^\dagger_j(t') + \hat{a}^\dagger_j(t')\hat{a}_i(t)\rangle, \tag{4.73}$$

where

$$\hat{a}(t) = e^{i\hat{H}t}\hat{a}e^{-i\hat{H}t} \tag{4.74}$$

obeys the equation of motion

$$i\hbar\partial_t\hat{a}(t) = [\hat{a}(t), \hat{H}]. \tag{4.75}$$

It turns out that G^R is only a function of $t - t'$. Thus it suffices to consider

$$G^R_{ij}(t) = G^R_{ij}(t, 0), \tag{4.76}$$

where we have set $t' = 0$.

4.5.1. For our case

$$\hat{H} = \sum_{ij} H_{ij}\hat{a}^\dagger_i\hat{a}_j. \tag{4.77}$$

Find the equation of motion

$$i\hbar\partial_t\hat{a}_i(t) = ????. \tag{4.78}$$

Solution 4.5.1. The basic rule is that

$$\begin{aligned} [a, bc] &= abc - bca && (4.79)\\ &= (ab + ba)c - b(ac + ca) && (4.80)\\ &= \{a, b\}c - b\{a, c\}. && (4.81) \end{aligned}$$

The only non-zero anticommutator will be between the creation and annihilation operator – which gives a delta function. Hence

$$i\hbar\partial_t\hat{a}_i(t) = \sum_j H_{ij}a_j(t). \tag{4.82}$$

4.5.2. For $t > 0$, use the last result to find the equation of motion for $G^R_{ij}(t)$. Note: the act of taking a derivative commutes with the act of taking an expectation value.

Solution 4.5.2. For $t > 0$ we can neglect the step function and

$$\begin{aligned} i\hbar\partial_t G^R_{ij}(t) &= i\hbar\partial_t \left[\frac{1}{i\hbar}\langle\hat{a}_i(t)\hat{a}^\dagger_j(0) + \hat{a}^\dagger_j(0)\hat{a}_i(t)\rangle\right] && (4.83)\\ &= \sum_k H_{ik}\left[\frac{1}{i\hbar}\langle\hat{a}_k(t)\hat{a}^\dagger_j(0) + \hat{a}^\dagger_j(0)\hat{a}_k(t)\rangle\right] && (4.84)\\ &= \sum_k H_{ik}G^R_{kj}(t) && (4.85) \end{aligned}$$

4.5.3. What is $G^R_{ij}(t = 0^+)$.

Solution 4.5.3.

$$G^R_{ij}(t = 0^+) = \frac{1}{i\hbar}\langle \hat{a}_i(0)\hat{a}^\dagger_j(0) + \hat{a}^\dagger_j(0)\hat{a}_i(0)\rangle \tag{4.86}$$

$$= \frac{1}{i\hbar}\delta_{ij}. \tag{4.87}$$

4.5.4. Combine these results to write an equation of motion for $G^R_{ij}(t)$ which is valid for all time. [This will be the same equation we worked with in class, so you know what to aim for.]

Solution 4.5.4. There are a number of ways to do this. One way is to note that for $t \neq 0$ the greens function obeys Eq. (4.85). We can then surmise that for some constant matrix A

$$i\hbar\partial_t G^R_{ij}(t) - \sum_k H_{ik}G^R_{kj}(t) = A_{ij}\delta(t). \tag{4.88}$$

Integrating this from $t = -\eta$ to $t = \eta$ yields

$$i\hbar[G^R_{ij}(\eta) - G^R_{ij}(-\eta)] = A_{ij}. \tag{4.89}$$

Hence $A_{ij} = \delta_{ij}$

4.5.5. Show that the function

$$G_{ij}(t) = \frac{1}{i}\theta(t)\langle \hat{a}_i(t)\hat{a}^\dagger_j\rangle - \frac{1}{i}\theta(-t)\langle \hat{a}^\dagger_j\hat{a}_i(t)\rangle \tag{4.90}$$

obeys the same equation of motion – and is also a Greens function (clearly with different boundary conditions however). This connection motivates the notation (which we will use in a future class)

$$G^>_{ij}(t) = \langle \hat{a}_i(t)\hat{a}^\dagger_j\rangle \tag{4.91}$$

$$G^<_{ij}(t) = \langle \hat{a}^\dagger_j\hat{a}_i(t)\rangle. \tag{4.92}$$

Despite using the symbol G, the functions $G^<$ and $G^>$ are not actually Greens functions – rather they are correlation functions.

Solution 4.5.5. Away from $t = 0$ this function obeys the same equation. The discontinuity at $t = 0$ is also the same. Thus it must obey the same equation everywhere.

Chapter 5

Calculating Greens Functions for Infinite Systems – Feb 7, 2018

Today we will develop the technology for calculating Greens functions by looking at a couple iconic examples. We will first explore a model of a semi-infinite wire, which will be the basis for our models of leads. We will then return to the notion of a self-energy, and see how it is used to calculate Greens functions for devices attached to leads.

A. Semi-Infinite 1D wire

The simplest model I can think of for a wire is

$$\hat{H} = -J \sum_j \left(\hat{a}_{j+1}^\dagger \hat{a}_j + \hat{a}_j^\dagger \hat{a}_{j+1} \right). \tag{5.1}$$

A semi-infinite wire is formed by putting bounds on the sum

$$\hat{H} = -J \sum_{j=0}^{\infty} \left(\hat{a}_{j+1}^\dagger \hat{a}_j + \hat{a}_j^\dagger \hat{a}_{j+1} \right). \tag{5.2}$$

In the obvious basis this can be represented by an infinite dimensional matrix H_{ij} which is zero unless i and j differ by 1.

Lets calculate $G_{00}(\omega)$, the matrix element of the Greens function evaluated at the first site. Physically this will be very useful. First, if we attach this wire to a device, the device will only know about things which are happening on that

first site. It will all be encoded in G_{00}. Second, it can tell us about the spectral density at that site.

Recall that

$$G_{ij} = \sum_\alpha \frac{(\psi_i^\alpha) * \psi_j^\alpha}{\omega - E_\alpha}. \tag{5.3}$$

where ψ^α is the eigenstate of H with energy E_α. Thus

$$G_{ii} = \sum_\alpha \frac{|\psi_i^\alpha|^2}{\omega - E_\alpha}. \tag{5.4}$$

The imaginary part of G_{ii} is then

$$A_{ii} = 2\mathrm{Im}G_{ii} = \sum_\alpha |\psi_i^\alpha|^2 2\pi\delta(\omega - E_\alpha). \tag{5.5}$$

This has the meaning of the density of modes on site i with energy ω. You can measure this quantity via tunneling spectroscopy.

I will make the argument in such a way that we can reuse it later for a more complicated problem. In particular, we break H into four pieces: H_0, H_s, Λ and $\Lambda^\dagger$. The first part H_0 describes the portion of the system for which we need the Greens function. It is the Hamiltonian projected into the space of interest. In this case, the projection just involves a single site,

$$H_0 = |0\rangle\langle 0|H|0\rangle\langle 0|. \tag{5.6}$$

Of course for us $H_0 = 0$. The second part H_s describes the portion of the system which is completely disjoint from the region of interest:

$$H_s = -J\sum_{j=1}^{\infty}\left(\hat{a}_{j+1}^\dagger \hat{a}_j + \hat{a}_j^\dagger \hat{a}_{j+1}\right). \tag{5.7}$$

Finally, Λ and $\Lambda^\dagger$ respectively contain the terms which take us out of and into the region of interest,

$$\Lambda = -Ja_0^\dagger a_1 \tag{5.8}$$

$$\Lambda^\dagger = -Ja_1^\dagger a_0. \tag{5.9}$$

These represents block in the matrix representation of H – and we can write

$$H = \begin{pmatrix} H_0 & \Lambda^\dagger \\ \Lambda & H_s \end{pmatrix}. \tag{5.10}$$

The top left block is 1×1. The bottom right is $\infty \times \infty$. The others are $1 \times \infty$ and $\infty \times 1$. Of course, in this basis those off-diagonal blocks have only one non-zero matrix element. Finally we introduce a projector

$$P_0 = |0\rangle\langle 0|. \tag{5.11}$$

As a projector $P_0^2 = P_0$ and $(1-P_0)^2 = (1-P_0)$.

The Greens function we want to calculate is

$$G = P_0 \frac{1}{E-H} P_0. \tag{5.12}$$

Problem 5.1.

5.1.1. Consider two matrices A and B, show that

$$\frac{1}{A+B} = \frac{1}{A}\frac{1}{1+BA^{-1}}. \tag{5.13}$$

Hint: Use that $(XY)^{-1} = Y^{-1}X^{-1}$.

Solution 5.1.1. This is straightforward:

$$\frac{1}{A+B} = \frac{1}{(1+BA^{-1})A} \tag{5.14}$$

$$= \frac{1}{A}\frac{1}{1+BA^{-1}}. \tag{5.15}$$

5.1.2. Use that result to write

$$\frac{1}{E-H} = \frac{1}{E-H_0-H_s}\frac{1}{1-XXX}. \tag{5.16}$$

Find XXX.

Solution 5.1.2.

$$\frac{1}{E-H_0-H_s-\Lambda-\Lambda^\dagger} = \frac{1}{E-H_0-H_s}\frac{1}{1-(\Lambda+\Lambda^\dagger)\frac{1}{E-H_0-H_s}} \tag{5.17}$$

5.1.3. Show that

$$P_0\frac{1}{E-H_0-H_s} = \frac{1}{E-H_0-H_s}P_0 = \frac{1}{E-H_0}P_0 = P_0\frac{1}{E-H_0}. \tag{5.18}$$

Solution 5.1.3. These result simply follow from the fact that $P_0H_s = H_sP_0 = 0$ and $P_0H_0 = H_0P_0 = H_0$.

5.1.4. Show that

$$(1-P_0)\frac{1}{E-H_0-H_s} = \frac{1}{E-H_0-H_s}(1-P_0) = \frac{1}{E-H_s}(1-P_0) = (1-P_0)\frac{1}{E-H_s}. \tag{5.19}$$

Solution 5.1.4. Same argument.

5.1.5. Show that

$$(\Lambda+\Lambda^\dagger)P_0 = (1-P_0)\Lambda = \Lambda \tag{5.20}$$

and

$$(\Lambda+\Lambda^\dagger)(1-P_0) = P_0\Lambda^\dagger = \Lambda^\dagger \tag{5.21}$$

Solution 5.1.5. Same argument.

5.1.6. We can Taylor expand the result in question 5.1.2 to formally write

$$G = P_0 \frac{1}{E - H} P_0 = P_0 \frac{1}{E - H_0 - H_s} \sum_{j=0}^{\infty} \left[(\Lambda + \Lambda^\dagger) \frac{1}{E - H_0 - H_s} \right]^j P_0. \quad (5.22)$$

Show that the $j = 1$ term of this series vanishes. What other j's will give terms which vanish?

Solution 5.1.6. The $j = 1$ term is

$$G_{j=1} = P_0 \frac{1}{E - H_0 - H_s} (\Lambda + \Lambda^\dagger) \frac{1}{E - H_0 - H_s} P_0. \quad (5.23)$$

We walk the P_0's through to get

$$G_{j=1} = \frac{1}{E - H_0} P_0 (\Lambda + \Lambda^\dagger) P_0 \frac{1}{E - H_0}. \quad (5.24)$$

But

$$P_0 (\Lambda + \Lambda^\dagger) P_0 = 0. \quad (5.25)$$

The same argument will make any odd j term vanish.

5.1.7. Simplify the $j = 2$ term by moving the P_0 through from right to left.

Solution 5.1.7. The $j = 2$ term is

$$G_{j=2} = P_0 \frac{1}{E - H_0 - H_s} (\Lambda + \Lambda^\dagger) \frac{1}{E - H_0 - H_s} (\Lambda + \Lambda^\dagger) \frac{1}{E - H_0 - H_s} P_0. \quad (5.26)$$

We walk the P_0's through to get

$$\begin{aligned}
G_{j=2} &= P_0 \frac{1}{E - H_0 - H_s} (\Lambda + \Lambda^\dagger) \frac{1}{E - H_0 - H_s} (\Lambda + \Lambda^\dagger) \frac{1}{E - H_0 - H_s} P_0 && (5.27)\\
&= P_0 \frac{1}{E - H_0 - H_s} (\Lambda + \Lambda^\dagger) \frac{1}{E - H_0 - H_s} (\Lambda + \Lambda^\dagger) P_0 \frac{1}{E - H_0} && (5.28)\\
&= P_0 \frac{1}{E - H_0 - H_s} (\Lambda + \Lambda^\dagger) \frac{1}{E - H_0 - H_s} (1 - P_0) \Lambda \frac{1}{E - H_0} && (5.29)\\
&= P_0 \frac{1}{E - H_0 - H_s} (\Lambda + \Lambda^\dagger) (1 - P_0) \frac{1}{E - H_s} \Lambda \frac{1}{E - H_0} && (5.30)\\
&= P_0 \frac{1}{E - H_0 - H_s} P_0 \Lambda^\dagger \frac{1}{E - H_s} \Lambda \frac{1}{E - H_0} && (5.31)\\
&= P_0 \frac{1}{E - H_0} \Lambda^\dagger \frac{1}{E - H_s} \Lambda \frac{1}{E - H_0}. && (5.32)
\end{aligned}$$

5.1.8. Show that

$$G = P_0 \frac{1}{1 - H_0} \sum_{j=0^\infty} \left[\Lambda^\dagger \frac{1}{E - H_s} \Lambda \frac{1}{E - H_0} \right]^j P_0 \quad (5.33)$$

Solution 5.1.8. This is the same argument applied to a general term.

5.1.9. Resum the series.

Solution 5.1.9.

$$G = P_0 \frac{1}{1-H_0} \frac{1}{1-\Lambda^\dagger \frac{1}{E-H_s} \Lambda \frac{1}{E-H_0}} P_0 \tag{5.34}$$

5.1.10. Use the result in question 5.1.2 to arrive at

$$G_{00} = \frac{1}{E - H_0 - \Sigma} \tag{5.35}$$

Find Σ. This result is generic, and did not use the specific form of H.

Solution 5.1.10.

$$G_{00} = P_0 \frac{1}{E - H_0 - \Lambda^\dagger \frac{1}{E-H_s} \Lambda} P_0 \tag{5.36}$$

so

$$\Sigma = \Lambda^\dagger \frac{1}{E-H_s} \Lambda \tag{5.37}$$

5.1.11. We can now specialize to the problem at hand, and note that

$$\Lambda_s^\dagger \frac{1}{E-H_s} \Lambda_s = J^2 |0\rangle\langle 1| \frac{1}{E-H_s} |1\rangle\langle 0|. \tag{5.38}$$

But

$$\langle 1| \frac{1}{E-H_s} |1\rangle = \langle 0| \frac{1}{E-H} |0\rangle = G_{00}. \tag{5.39}$$

Thus

$$G_{00} = \frac{1}{E - J^2 G_{00}}. \tag{5.40}$$

Solve this equation for G_{00}.

Solution 5.1.11. This is a quadratic equation.

$$J^2 G_{00}^2 - E G_{00} + 1 = 0, \tag{5.41}$$

with solution

$$G_{00} = \frac{E}{2J^2} \pm \sqrt{\frac{E^2}{4J^4} - 1}. \tag{5.42}$$

For the retarded Greens function we want the + branch. The structure is explored in the homework.

5.1.12. Calculate the spectral density $A_{00}(E) = 2\mathrm{Im} G_{00}(E)$. For what values of E is the spectral density non-zero?

Solution 5.1.12. The spectral density will be non-zero if $-2J < E < 2J$. This is sensible, because the eigenstates of an infinite wire all are in this range. One then finds that the spectral density is a semi-circle,

$$A(E) = \sqrt{4 - \frac{E^2}{J^2}}. \tag{5.43}$$

A.1. Comments

This is a nice example, because it is non-trivial, and computationally clean. This is one of the better ways of calculating the spectral density on the first site of an open chain. We also once again saw the "Self-Energy," Σ, which encoded how the rest of the wire influences the wavefunction on the first site.

B. Infinite Wire

We will now use this tricky result (the Greens function for a semi-infinite wire) to calculate a well-known result – the density of states of an infinite wire. We will do this as an example of how to analyze a device with leads: we will interpret our wire as single site, with two semi-infinite leads attached to it. Thus

$$H = H_0 + (H_L + \Lambda_L + \Lambda_L^\dagger) + (H_R + \Lambda_R + \Lambda_R^\dagger). \tag{5.44}$$

Where H_0 contains terms which only act on the site $j = 0$ (which is $H_0 = 0$ yet again). The other terms are

$$\begin{aligned} H_R &= -J\sum_{j=1}^{\infty}(a_j^\dagger a_{j+1} + a_{j+1}^\dagger a_j) && (5.45)\\ H_L &= -J\sum_{j=-\infty}^{-1}(a_j^\dagger a_{j-1} + a_{j-1}^\dagger a_j) && (5.46)\\ \Lambda_R &= -Ja_0^\dagger a_1 && (5.47)\\ \Lambda_L &= -Ja_0^\dagger a_{-1}. && (5.48) \end{aligned}$$

The same argument that we used previously gives

$$G = \frac{1}{E - H_0 - \Sigma_L - \Sigma_R} \tag{5.49}$$

where

$$\begin{aligned} \Sigma_L &= J^2 G_L && (5.50)\\ \Sigma_R &= J^2 G_R && (5.51) \end{aligned}$$

with G_L and G_R the greens function for the first site of each lead, assuming you separated it from the system. In this case

$$G_L = G_R = \frac{E}{2J^2} + \sqrt{\frac{E^2}{4J^4} - 1} \tag{5.52}$$

Thus we find

$$\begin{aligned} G &= \frac{1}{E - 2J^2\left[\frac{E}{2J^2} + \sqrt{\frac{E^2}{4J^4} - 1}\right]} && (5.53)\\ &= \frac{1}{-\sqrt{E^2 - J^2}}. && (5.54) \end{aligned}$$

The density of states is then

$$\begin{aligned} A(E) &= 2\mathrm{Im}G && (5.55)\\ &= \frac{2}{\sqrt{4J^2 - E^2}} && (5.56) \end{aligned}$$

In homework you will verify that this agrees with more conventional arguments. You might remember that in 1D the density of states goes as $1/\sqrt{E}$ This also emerges here since:

$$\frac{2}{\sqrt{4J^2 - E^2}} = \frac{2}{\sqrt{2J - E}\sqrt{2J + E}} \tag{5.57}$$

If E is near $-2J$, then

$$A(E) \approx \frac{2}{\sqrt{4J}}\frac{1}{\sqrt{2J + E}} \tag{5.58}$$

C. Beyond 1D

A more general wire is made of repeating units of M sites. For example, we could have a rectangular strip which is M sites wide. Here we will explain how to find the $M \times M$ matrix which represents the Greens function for that first cell.

We let H^0_{ij} be the matrix elements of the Hamiltonian in that first layer. We let $\Lambda_{\bar{i}j}$ be the matrix elements of the Hamiltonian between the sites $\bar{i}$ in the second layer and sites j in this first layer. Finally let $\bar{G}_{\bar{i}\bar{j}}$ be the Greens function of the lead if we removed the first layer – this time taking $\bar{i}, \bar{j}$ to lie in the second layer. By translational invariance $\bar{G} = G$. This equality was the crux of how we calculated the Greens function in section A.

What happens if the Hamiltonian has next nearest neighbor hopping? Well, then we just combine the first two rows into one – and call that the first layer.

Thus if we have a strip of width M with next-nearest-neighbor hopping, we will need a $2M \times 2M$ matrix to represent H^0.

Being careful with our matrix multiplication, our previous argument goes through, and we find

$$G = \frac{1}{E - H^0 - \Lambda^\dagger \bar{G} \Lambda}. \tag{5.59}$$

Identifying $\bar{G} = G$, this can be written as a quadratic equation

$$\Lambda^\dagger G \Lambda G - (E - H^0)G + 1 = 0, \tag{5.60}$$

where 1 is the identity matrix.

Equations like Eq. (5.60) are straightforward if Λ commutes with H^0, in which case one simply works in the basis that simultaneously diagonalizes Λ and H^0. Unfortunately, here they don't commute. Aside from numerical iteration, the main approach to solving these nonlinear operator equations involves a transfer matrix approach. I will leave this approach as an exercise in the homework.

D. Spectral Representation of Self-Energy

The Self-Energy is generically

$$\hat{\Sigma} = \Lambda^\dagger \frac{1}{\omega - \hat{G}_{\text{lead}}} \Lambda. \tag{5.61}$$

It is convenient to write this in terms of the eigenvalues $|\alpha\rangle$ of G_{lead}, corresponding to the energy eigensates of an isolated lead

$$\hat{\Sigma} = \sum_\alpha \Lambda^\dagger |\alpha\rangle \frac{1}{\omega - E_\alpha} < \alpha|\Lambda. \tag{5.62}$$

The imaginary part of Σ is related to the spectral density

$$\Gamma = \frac{\Sigma - \Sigma^\dagger}{i} = \sum_\alpha \Lambda^\dagger |\alpha\rangle 2\pi\delta(\omega - E_\alpha)\langle\alpha|\Lambda. \tag{5.63}$$

The homework has a concrete example.

E. Homework

Problem 5.2. Response to periodic perturbation

5.2.1. Consider a Schrodinger equation driven by an a periodic external perturbation:

$$i\hbar\partial_t \psi(t) - H\psi(t) = f e^{-i\nu t}. \tag{5.64}$$

Fourier transform this equation to produce an equation for $\psi(\omega)$.

Solution 5.2.1.

$$(\hbar\omega - H)\,\psi(\omega) = f\delta(\omega - \nu) \tag{5.65}$$

5.2.2. Solve for $\psi(\omega)$. Relate the solution to the Greens function $G^R(\omega)$.

Solution 5.2.2.

$$\begin{aligned} \psi(\omega) &= \frac{1}{\hbar\omega - H} f\delta(\omega - \nu) && (5.66)\\ &= G^R(\omega) f\delta(\omega - \nu). && (5.67) \end{aligned}$$

Problem 5.3. Greens function for a simple quantum dot attached to 1D leads

Consider a simple model for a quantum dot attached to 1D leads, namely

$$H = \epsilon_0 \hat{a}_0^\dagger \hat{a}_0 + \sum_{j=-\infty}^{\infty} -J(a_j^\dagger a_{j+1} + a_{j+1}^\dagger a_j). \tag{5.68}$$

5.3.1. Treat the $j = 0$ site as the "system," and the sites with $j > 0$ and $j < 0$ as the right and left leads. What is

$$H_0 \tag{5.69}$$
$$H_L \tag{5.70}$$
$$H_R \tag{5.71}$$
$$\Lambda_L \tag{5.72}$$
$$\Lambda_R \tag{5.73}$$
$$\Sigma_L \tag{5.74}$$
$$\Sigma_R \tag{5.75}$$
$$\Gamma_L \tag{5.76}$$
$$\Gamma_R \tag{5.77}$$

Solution 5.3.1.

$$H_0 = \epsilon_0 a_0^\dagger a_0 \tag{5.78}$$
$$H_L = \sum_{j<0} -J(a_j^\dagger a_{j-1} + a_{j-1}^\dagger a_j) \tag{5.79}$$
$$H_R = \sum_{j>0} -J(a_j^\dagger a_{j+1} + a_{j+1}^\dagger a_j) \tag{5.80}$$
$$\Lambda_L = -J a_0^\dagger a_{-1} \tag{5.81}$$
$$\Lambda_R = -J a_0^\dagger a_1 \tag{5.82}$$
$$\Sigma_L = J\left[\frac{E}{2J} + \sqrt{\frac{E^2}{4J^2} - 1}\right] \tag{5.83}$$
$$\Sigma_R = J\left[\frac{E}{2J} + \sqrt{\frac{E^2}{4J^2} - 1}\right] \tag{5.84}$$
$$\Gamma_L = J\sqrt{1 - \frac{E^2}{4J^2}} \tag{5.85}$$
$$\Gamma_R = J\sqrt{1 - \frac{E^2}{4J^2}} \tag{5.86}$$

5.3.2. What is the Greens function for the site?

Solution 5.3.2.

$$G = \frac{1}{E - H_0 - \Sigma_L - \Sigma_R} \tag{5.87}$$
$$= \frac{1}{-\epsilon_0 - \sqrt{E^2 - 4J^2}} \tag{5.88}$$

5.3.3. What is the spectral density for the site?

Solution 5.3.3. If $|E| < 2J$ things are simple, and

$$A = \frac{G^\dagger - G}{i} \tag{5.89}$$
$$= \frac{1}{i}\left[\frac{1}{-\epsilon_0 + i\sqrt{4J^2 - E^2}} - \frac{1}{-\epsilon_0 - i\sqrt{4J^2 - E^2}}\right] \tag{5.90}$$
$$= \frac{2\sqrt{4J^2 - E^2}}{\epsilon_0^2 + 4J^2 - E^2} \tag{5.91}$$

Solution 5.3.3. It turns out that this result is incomplete, as the Greens function can have discrete poles when $|E| > 2J$. I didn't talk about this in class, so I don't expect anyone to do it – but it is useful to give the argument here. Normally I wouldn't be so formal, but I will try to be pedagogical here. Note: these poles represent bound states, so they will not contribute to transport.

Firstly, we need to be a bit more careful about our branch cuts. The branch we actually want is the principle branch of

$$G = \frac{1}{-\epsilon_0 - i\sqrt{4J^2 - (E + i\eta)^2}}, \tag{5.92}$$

as $\eta \to 0^+$. For $-2J < E < 2J$ this is just what we had before. For $E > 2J$ we will be taking the square root of a number with a negative real part and a very small negative imaginary part. Thus the square root gives us a $-i$ and we have

$$G(E > 2J) = \frac{1}{-\epsilon_0 - \sqrt{E^2 - 4J^2}}. \tag{5.93}$$

For $E < -2J$ we will be taking the square root of a number with a negative real part and a very small positive imaginary part. Thus the square root gives us $+i$ and we have

$$G(E < -2J) = \frac{1}{-\epsilon_0 + \sqrt{E^2 - 4J^2}}. \tag{5.94}$$

Thus when $\epsilon_0 < 0$ there is a pole at $E < -2J$, and when $\epsilon_0 > 0$ there is a pole at $E > 2J$. The pole will be located at

$$E^2 = 4J^2 + \epsilon_0^2. \tag{5.95}$$

Solution 5.3.3. Lets first treat the case $\epsilon_0 > 0$, in which case we define

$$E_0 = \sqrt{4J^2 + \epsilon_0^2}, \tag{5.96}$$

and to find the residue write

$$E = E_0 + \delta E \tag{5.97}$$

with δE small. The greens function is then

$$\begin{aligned} G &\approx \frac{1}{-\epsilon_0 - \sqrt{E_0^2 - 4J^2 + 2E_0\delta E}} && (5.98)\\ &\approx \frac{1}{-\epsilon_0 - \sqrt{E_0^2 - 4J^2} - E_0\delta E/\sqrt{E_0^2 - 4J^2}} && (5.99)\\ &= \frac{1}{-E_0\delta E/\epsilon_0} && (5.100)\\ &= \frac{-\epsilon_0/E_0}{E - E_0}, && (5.101) \end{aligned}$$

which gives a contribution to the spectral density of

$$A = \frac{\epsilon_0}{\sqrt{4J^2 + \epsilon_0^2}} 2\pi\delta(E - E_0). \tag{5.102}$$

In particular if $\epsilon_0 \gg 2J$, one can ignore the leads, and the spectral density is just a single delta function at $E = \epsilon_0$.
One finds a similar expression for $\epsilon_0 < 0$, But in that case the pole is at negative E.
If one is not careful about these branch cuts one might accidentally believe there are two poles. A sure way to guard against this is to think about what happens when ϵ_0 is very large. It is clearly unphysical to have a pole at $E = -\epsilon_0$.

Problem 5.4. Conventional calculation of density of states

5.4.1. A 1D wire has a dispersion $\epsilon_k = -2t\cos(k)$. Each of these states are spatially homogeneous, with density $1/L$. Thus the density of states will be

$$\begin{aligned} \rho(E) &= \sum_k \frac{1}{L} 2\pi\delta(E - \epsilon_k) && (5.103)\\ &= \int_{-\pi}^{\pi} \frac{dk}{2\pi} 2\pi\delta(E + 2t\cos(k)) && (5.104)\\ &= 2\int_0^{\pi} dk\, \delta(E + 2t\cos(k)). && (5.105) \end{aligned}$$

Carry out the integral to calculate the density of states. How does it compare to the results that we arrived at in class?

Solution 5.4.1.

$$\rho(E) = 2\int_0^\pi dk\, \frac{\delta(k + \arccos E/(2t))}{2t\sin(k)} \tag{5.106}$$

We then do some trigonometry. If $\cos(k) = -E/(2t)$, then $\sin(k) = \sqrt{4t^2 - E^2}/(2t)$, and we get

$$\rho(E) = \frac{2}{\sqrt{4t^2 - E^2}} \tag{5.107}$$

which coincides with what we found with Greens functions.

5.4.2. For a finite 1D chain of length L, with sites $j = 1, 2, \cdots L$, the normalized eigenstates are

$$\psi_j = \frac{\sqrt{2}}{\sqrt{L}}\sin(kj), \tag{5.108}$$

where

$$k = \frac{n\pi}{L+1}, \tag{5.109}$$

with $n = 1, 2, \cdots L$. Again the energy is $\epsilon_k = -2t\cos(k)$.

Calculate the local density of states at the first site of the chain (in the limit $L \to \infty$). Compare to the result we derived in class.

Solution 5.4.2.

$$\rho_1(E) = L\int \frac{dk}{2\pi}|\psi_1|^2 2\pi\delta(E - \epsilon_k) \tag{5.110}$$

$$= 4\int_0^\pi dk\, \sin^2(k)\delta(E + 2t\cos(k)) \tag{5.111}$$

$$= 4\int_0^\pi dk\, \frac{\sin(k)}{2t}\delta(k + \arccos E/(2t)) \tag{5.112}$$

$$= \frac{4}{2t}\frac{\sqrt{4t^2 - E^2}}{2t} \tag{5.113}$$

$$= \frac{1}{t}\sqrt{4 - \frac{E^2}{t^2}}. \tag{5.114}$$

Problem 5.5. Formal Properties of Greens Functions This question is a bit abstract, and is not actually needed for this course – but it is good mathematical background.

5.5.1. Analytic Properties – Discontinuities across the real axis

Consider a function

$$G(\omega) = \int_{-\infty}^{\infty} \frac{dz}{2\pi} \frac{1}{\omega - z} A(z), \tag{5.115}$$

where $A(z)$ is an arbitrary real valued function, and the integral is taken over the real z-axis.

Use the expression that for real x

$$\frac{1}{x \pm i\eta} = \frac{P}{x} \mp i\pi\delta(x) \tag{5.116}$$

To show that $G(\omega)$ is discontinuous across the real ω axis and find the discontinuity

$$G(\omega + i\eta) - G(\omega - i\eta) \tag{5.117}$$

for real ω.

It turns out that G is continuous everywhere except the real axis. Generically the discontinuity corresponds to a Branch Cut – and one can define $G^R(\omega)$ to be the analytic continuation from the upper half plane, and $G^A(\omega)$ to be the analytic continuation from the lower half-plane.

Solution 5.5.1. This is straightforward.

5.5.2. Kramers-Kronig – part 1 Take ω real. Use Eq. (5.115) and Eq. 5.116 to express the real part of $G^R(\omega) = G(\omega + i\eta)$ as a principle-value integral of the imaginary part of $G^R(\omega)$.

This is the first half of the Kramers-Kronig relations.

Solution 5.5.2. This is again straightforward

$$\begin{aligned} \mathrm{Re}G^R(\omega) &= \mathrm{Re} \int \frac{dz}{2\pi} \frac{1}{\omega - z} A(z) && (5.118) \\ &= P \int \frac{dz}{2\pi} \frac{A(z)}{\omega - z} && (5.119) \\ &= \frac{1}{\pi} P \int \frac{dz}{\omega - Z} \mathrm{Im}G^R(z). && (5.120) \end{aligned}$$

5.5.3. Kramers-Kronig – part 2 To get the full Kramers-Kronig relations, we note that if $G^R(\omega)$ is analytic in the upper half plane, then for any closed contour Γ in the upper half plane

$$\oint_\Gamma \frac{d\omega}{2\pi} \frac{G^R(\omega)}{z - \omega} = 0. \tag{5.121}$$

In particular we take a contour that skims along the real axis, then is closed by a half-circle in the upper-half plane.

It is obvious from Eq. (5.115) that $G^R(\omega)$ vanishes when the imaginary part of ω is large. Thus the integral over the half circles vanish, and one must have

$$\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{G^R(\omega)}{z-\omega} = 0. \tag{5.122}$$

Take the real and imaginary part of this equation to derive two integral equations relating the real and imaginary part of G^R. One of them should coincide with the equation you found in question 5.5.2.

Solution 5.5.3. First the real part:

$$\begin{aligned} \mathrm{Re}\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{G^R(z)}{z-\omega+i\eta} &= P\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{\mathrm{Re}G^R(z)}{z-\omega} \\ &\quad + \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \mathrm{Im}G^R(z)\pi\delta(z-\omega) \\ &= P\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{\mathrm{Re}G^R(z)}{z-\omega} + \frac{1}{2}\mathrm{Im}G^R(\omega). \end{aligned} \tag{5.123}$$

Next the imaginary part:

$$\begin{aligned} \mathrm{Im}\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{G^R(z)}{z-\omega+i\eta} &= P\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{\mathrm{Im}G^R(z)}{z-\omega} \\ &\quad - \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \mathrm{Re}G^R(z)\pi\delta(z-\omega) \\ &= P\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{\mathrm{Im}G^R(z)}{z-\omega} - \frac{1}{2}\mathrm{Re}G^R(\omega). \end{aligned} \tag{5.124}$$

Setting each of these to zero gives the Kramers-Kronig relations

$$\mathrm{Re}G^R(\omega) = \frac{1}{\pi} P\int_{-\infty}^{\infty} \frac{d\omega}{z-\omega} \mathrm{Im}G^R(z) \tag{5.125}$$

$$\mathrm{Im}G^R(\omega) = -\frac{1}{\pi} P\int_{-\infty}^{\infty} \frac{d\omega}{z-\omega} \mathrm{Re}G^R(z) \tag{5.126}$$

Problem 5.6. A more complicated 1D lead

Here we try to calculate the Greens function for a semi-infinite wire with a non-trivial unit cell. Following the arguments of section C, we break the wire up into layers – each of which contain M sites. The Hamiltonian contains matrix elements within each layer. In the main text we referred to this $M \times M$ matrix as H^0. To save some ink, here we will just refer to it as H. There is also a $M \times M$ matrix Λ which contains the elements of the Hamiltonian which connect two sequential layers.

This problem is a bit heavy – and in practice we will not do this by hand – this algorithm (or some equivalent) is built into Kwant. It is kind of fun to go through this though. Don't sweat it if you get lost.

5.6.1. As a concrete example, you can imagine a lead which is two-sites wide. One might then write

$$H = \begin{pmatrix} 0 & -t \\ -t & 0 \end{pmatrix} \tag{5.127}$$

$$\Lambda = \begin{pmatrix} -t & 0 \\ 0 & -t \end{pmatrix} \tag{5.128}$$

In this case Λ and H commute, so one can solve Eq. (5.60) by going into the basis which diagonalizes H.

Find the Greens function for the first layer of the lead in this simple case. It will be a 2×2 matrix.

Solution 5.6.1. The eigenvectors and eigenvalues are

$$\psi_1 = \begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix} \quad \epsilon_1 = -J \tag{5.129}$$

$$\psi_2 = \begin{pmatrix} 1/\sqrt{2} \\ -1/\sqrt{2} \end{pmatrix} \quad \epsilon_2 = J \tag{5.130}$$

These are also eigenvectors of Λ with eigenvalue $\lambda = -t$.
We need to solve the equation

$$\Lambda^\dagger G \Lambda G - (E - H^0)G + 1 = 0. \tag{5.131}$$

The matrix G will be diagonal in this same basis, with eigenvalues g_1 and g_2 that solve

$$\lambda^2 g_j^2 - (E - \epsilon_j)g_j + 1 = 0. \tag{5.132}$$

which gives

$$g_j = \frac{E - \epsilon_j}{2} + \sqrt{(E - \epsilon_j)^2 - 4\lambda^2}. \tag{5.133}$$

The matrix is then

$$G = \psi_1 g_1 \psi_1^\dagger + \psi_2 g_2 \psi_2^\dagger \tag{5.134}$$

$$= \frac{1}{2}\begin{pmatrix} g_1 + g_2 & g_1 - g_2 \\ g_1 - g_2 & g_1 + g_2 \end{pmatrix} \tag{5.135}$$

5.6.2. As a second concrete example, imagine we have a 1D lead, but we have

next-nearest neighbor hopping,

$$H_{\text{lead}} = \sum_{j=1}^{\infty} \left[-t(a_j^\dagger a_{j+1} + a_{j+1}^\dagger a_j) - t'(a_j^\dagger a_{j+2} + a_{j+2}^\dagger a_j) \right]. \tag{5.136}$$

In this case one "layer" is two sites, and the Hamiltonian describing the first layer is

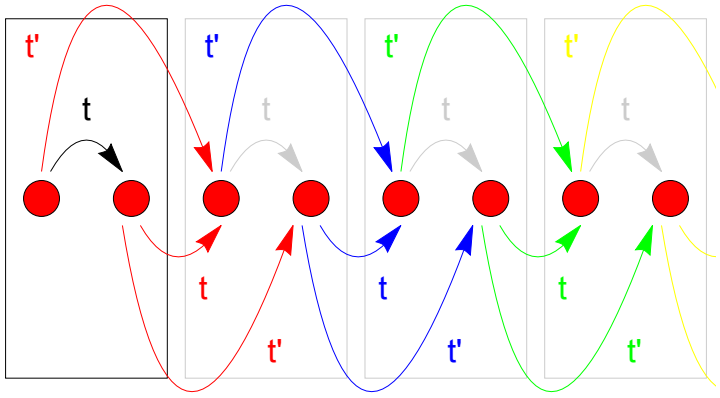
$$H = \begin{pmatrix} 0 & -t \\ -t & 0 \end{pmatrix}, \tag{5.137}$$

and the operator that connects layers is

$$\Lambda = \begin{pmatrix} -t' & -t \\ 0 & -t' \end{pmatrix}. \tag{5.138}$$

Draw a picture which illustrates the first 4 sites, with labeled arrows between them depicting the various hoppings. Then show that H and Λ do not commute.

Solution 5.6.2. Here is the first 8 sites:



The boxes show the different "layers". There is one hopping on the inside of each box, and three joining each subsequent layers. I drew "one-way" arrows, but the hoppings go in each direction.

The commutator is

$$[H, \Lambda] = \begin{pmatrix} -t^2 & 0 \\ 0 & t^2 \end{pmatrix}, \tag{5.139}$$

which is non-zero as long as $t \neq 0$.

5.6.3. Transfer Matrices In the case where $[H, \Lambda] \neq 0$ we need to do a trick which converts the solution of a quadratic eigenvalue equation to that of an auxilliary linear system. The argument is most transparent if we introduce matrices G_{ij}^{mn} which are the Greens functions between the m'th layer, i'th site,

and the n'th layer, j'th site. By definition

$$\begin{pmatrix} \omega - H & -\Lambda & 0 & \cdots \\ -\Lambda^\dagger & \omega - H & -\Lambda & \cdots \\ 0 & -\Lambda^\dagger & \omega - H & \cdots \\ \vdots & & & \end{pmatrix} \begin{pmatrix} G^{00} & G^{10} & \cdots & \cdots \\ G^{01} & G^{11} & \cdots & \\ \vdots & & & \\ \vdots & & & \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & \cdots \\ 0 & 1 & 0 & \cdots \\ 0 & 0 & 1 & \cdots \\ \vdots & & & \end{pmatrix}. \tag{5.140}$$

We take the first column of this equation and note that for $m > 1$,

$$\begin{aligned} \begin{pmatrix} G^{0m} \\ G^{0\,m+1} \end{pmatrix} &= \begin{pmatrix} 0 & 1 \\ -\Lambda^{-1}\Lambda^\dagger & XX \end{pmatrix} \begin{pmatrix} G^{0m-1} \\ G^{0\,m} \end{pmatrix} \\ &= T \begin{pmatrix} G^{0m-1} \\ G^{0\,m} \end{pmatrix}, \end{aligned} \tag{5.141}$$

which defines the transfer matrix T. Find XX.

Solution 5.6.3.

$$T = \begin{pmatrix} 0 & 1 \\ -\Lambda^{-1}\Lambda^\dagger & -\Lambda^{-1}(\omega - H) \end{pmatrix} \tag{5.142}$$

and

$$XX = -\Lambda^{-1}(\omega - H) \tag{5.143}$$

5.6.4. For the case of Eq. (5.137) find T. (Note, we are assuming t and t' are real.)

Solution 5.6.4. The inverse matrix is

$$\Lambda^{-1} = \begin{pmatrix} -\frac{1}{t'} & \frac{t}{(t')^2} \\ 0 & -\frac{1}{t'} \end{pmatrix} \tag{5.144}$$

Thus

$$T = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ -1 + \frac{t^2}{(t')^2} & \frac{t}{t'} & \frac{\omega}{t'} - \frac{t^2}{(t')^2} & \frac{t}{t'} - \frac{\omega t}{(t')^2} \\ -\frac{t}{t'} & -1 & \frac{t}{t'} & \frac{\omega}{t'} \end{pmatrix}. \tag{5.145}$$

5.6.5. Next we note that

$$(\omega - H)G^{00} + \Lambda G^{01} = 1 \tag{5.146}$$

or equivalently

$$\begin{pmatrix} G^{00} \\ G^{01} \end{pmatrix} = T \begin{pmatrix} XX \\ G^{00} \end{pmatrix}. \tag{5.147}$$

and hence

$$\begin{pmatrix} G^{0m-1} \\ G^{0\,m} \end{pmatrix} = T^m \begin{pmatrix} XX \\ G^{00} \end{pmatrix}. \tag{5.148}$$

Find XX.

Solution 5.6.5. It is easiest to multiply out EQ. (5.147), which becomes two equations

$$G^{00} = G^{00} \tag{5.149}$$
$$G^{01} = -\Lambda^{-1}\Lambda^\dagger XX - \Lambda^{-1}(\omega - H)G^{00}. \tag{5.150}$$

The first equation is a tautology. If we multiply the second by Λ we get

$$\Lambda G^{01} + (\omega - H)G^{00} = -\Lambda^\dagger XX. \tag{5.151}$$

Clearly this means $XX = -(\Lambda^\dagger)^{-1}$.

5.6.6. Show that

$$T^\dagger \Omega T = \Omega \tag{5.152}$$

where

$$\Omega = \begin{pmatrix} 0 & -\Lambda \\ \Lambda^\dagger & 0 \end{pmatrix} \tag{5.153}$$

is a skew-Hermitian matrix ($\Omega^\dagger = -\Omega$).

The property in Eq. 5.152 is described as "Symplectic." [Or sometimes "complex-symplectic" or "conjugate-sympectic" – as traditionally the symplectic condition involves the transpose of T rather than the Hermitian-Conjugate.]

5.6.7. Because of the symplectic property, the eigenvectors of T come in pairs. Let χ be an eigenvector of T with eigenvalue λ:

$$T\chi = \lambda\chi. \tag{5.154}$$

Use the symplectic property to show that $\Omega\chi$ is an eigenvector of $T^\dagger$ with eigenvalue $1/\lambda$.

The eigenvalues of a matrix are the complex conjugate of the eigenvalues of the Hermitian conjugate of a matrix. Thus we can conclude that if λ is an eigenvalue of T, then so is $1/\lambda^*$. Thus either $|\lambda| = 1$, or for every eigenvalue with modulus greater than unity there is one that is smaller.

To get the branch cuts right, we add a small positive imaginary part to ω. Formally this breaks the complex-symplectic structure, but it is restored as we take the imaginary part to zero. It turns out that once we add this imaginary part, none of the eigenvalues have unit magnitude. (You can see this by looking

at the determinant of $T^\dagger T - 1$, but I won't go into the argument.) In fact, with the infinitesmal imaginary part added, half the eigenvalues have modulus greater than 1, and half have modulus less than 1.

Solution 5.6.6. If $T\chi = \lambda\chi$, then $T^\dagger \Omega T \chi = \lambda T^\dagger \Omega \chi$. But by the symplectic condition $T^\dagger \Omega T \chi = \Omega\chi$. Thus

$$T^\dagger (\Omega\chi) = \frac{1}{\lambda} (\Omega\chi), \tag{5.155}$$

which is the desired result.

5.6.8. We denote the N eigenvalues which have modulus less than 1 as $\lambda_1, \lambda_2, \cdots \lambda_N$, and the corresponding eigenvectors $(\psi_1, \phi_1), (\psi_2, \phi_2), \cdots (\psi_N, \phi_N)$, as in

$$\begin{pmatrix} 0 & 1 \\ -\Lambda^{-1}\Lambda^\dagger & -\Lambda^{-1}(\omega + i\eta - H) \end{pmatrix} \begin{pmatrix} \psi_j \\ \phi_j \end{pmatrix} = \lambda_j \begin{pmatrix} \psi_j \\ \phi_j \end{pmatrix}. \tag{5.156}$$

These are readily found numerically.

For the case of Eq. (5.137) with $t = 0$ find the ψ_j and ϕ_j. [I used a computer algebra system – though you can do it by hand if you note that under this circumstance, T is block diagonal.] You can take $\eta \to 0$ once you have figured out which eigenvalues have modulus less than 1.

[Note the case $t = 0$ corresponds to when $[\Lambda, H] = 0$, so we could have solved this case directly using a more elementary approach. Moreover, in this case the even and odd sites decouple, so our lead is really two separate leads. Regardless, it is a good case to explore the arithmetic.]

Solution 5.6.7. The eigenvectors whose eigenvalues have magnitude less than 1 (when $\eta \neq 0$) are

$$\psi_1 = \begin{pmatrix} \frac{\omega + i\sqrt{4(t')^2 - \omega^2}}{2t'} \\ 0 \end{pmatrix} \tag{5.157}$$

$$\phi_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{5.158}$$

$$\lambda_1 = \frac{\omega - i\sqrt{4(t')^2 - \omega^2}}{2t'} \tag{5.159}$$

$$\psi_2 = \begin{pmatrix} 0 \\ \frac{\omega + i\sqrt{4(t')^2 - \omega^2}}{2t'} \end{pmatrix} \tag{5.160}$$

$$\phi_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{5.161}$$

$$\lambda_2 = \frac{\omega - i\sqrt{4(t')^2 - \omega^2}}{2t'}. \tag{5.162}$$

5.6.9. In order for the Greens functions in Eq. (5.148) to be bounded, we must have that the vector on the right hand side is only made from the (ψ_j, ϕ_j). That is

$$-(\Lambda^{-1})_{ij} = \sum_j c_{ij}\psi_{jk} \tag{5.163}$$

$$G^{00}_{ik} = \sum_j c_{ij}\phi_{jk}, \tag{5.164}$$

where ψ_{jk} is the k'th entry of the vector ψ_j. The previous version had an erroneous $\Lambda^\dagger$ in Eq. (5.163). Everything is known in Eq. (5.163) except the c's. Assuming the matrix of coefficients of the ψ's is invertible, we can immediately extract

$$c = -\Lambda^{-1}\psi^{-1} \tag{5.165}$$

and

$$G^{00} = c\psi = -\Lambda^{-1}\psi^{-1}\phi. \tag{5.166}$$

Since G^{00} is what we were trying to find, we are now done.

Use this approach to find G^{00} for the case of Eq. (5.137) with $t = 0$

Solution 5.6.8. The matrices are

$$\phi = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \tag{5.167}$$

$$\psi = \frac{\omega + i\sqrt{4(t')^2 - \omega^2}}{2t'} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \tag{5.168}$$

$$\psi^{-1} = \frac{\omega - i\sqrt{4(t')^2 - \omega^2}}{2t'} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \tag{5.169}$$

$$\Lambda^{-1} = \frac{-1}{t'} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \tag{5.170}$$

Thus

$$G = \frac{\omega + i\sqrt{4(t')^2 - \omega^2}}{2(t')^2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \tag{5.171}$$

Chapter 6

Calculating Transport from Greens Functions – Feb 9, 2018

We now finally have all the tools to calculate transport. Just to keep you from the suspense, the end result (in the absence of scattering) is that in linear-response we will find that the net current entering from lead s is

$$I_s = \sum_{s'} \sigma_{ss'} V_{s'}, \tag{6.1}$$

where $V_{s'}$ is the voltage applied to lead s', and the conductivity tensor is

$$\sigma_{ss'} = -\frac{q}{2\pi\hbar}\left[\mathrm{Tr}\Gamma^s G \Gamma^{s'} G^\dagger - \delta_{ss'} \sum_{\bar{s}} \mathrm{Tr}\Gamma^s G \Gamma^{\bar{s}} G^\dagger\right], \tag{6.2}$$

where $G = G^R = G(\omega + i\eta)$, $G^\dagger = G^A = G(\omega - i\eta)$, and $\Gamma^s = 2\mathrm{Im}\Sigma^s(\omega + i\eta)$. Today we will derive this expression, and figure out how to calculate currents inside the device.

In a typical device, some leads have known currents going down them, while other leads have known voltages. Typically the other quantity is unknown. For example, there are no currents going through the leads that go to a voltmeter. Thus one generically has some of the unknowns on the right hand side of Eq. (6.1) while others are on the left. This feature does not make the equations any harder to solve.

There are a few important physical properties of the conductivity matrix.

First, the total incoming current should vanish. Thus we look at

$$\sum_s I_s = \sum_{ss'} \sigma_{ss'} V_{s'}. \tag{6.3}$$

But if we sum Eq. (6.2) we find

$$-\frac{2\pi\hbar}{q}\sum_s \sigma_{ss'} \quad = \quad \sum_s \mathrm{Tr}\Gamma^s G\Gamma^{s'} G^\dagger - \sum_{\bar{s}} \mathrm{Tr}\Gamma^{s'} G\Gamma^{\bar{s}} G^\dagger, \tag{6.4}$$

which is zero because Γ is Hermitian. Second, it is only differences in voltages that matter. If we add a constant to all the voltages, the currents should not change. This is encoded in

$$-\frac{2\pi\hbar}{q}\sum_{s'} \sigma_{ss'} = \sum_{s'} \mathrm{Tr}\Gamma^s G\Gamma^{s'} G^\dagger - \sum_{\bar{s}} \mathrm{Tr}\Gamma^s G\Gamma^{\bar{s}} G^\dagger, \tag{6.5}$$

which is clearly zero.

Of course, this makes it clear that a more sensible way to write the result is

$$I_s = \sum_{s'} \bar{\sigma}_{ss'}(V_{s'} - V_s) \tag{6.6}$$

with

$$\bar{\sigma}_{ss'} = -\frac{q}{2\pi\hbar}\left[\mathrm{Tr}\Gamma^s G\Gamma^{s'} G^\dagger\right]. \tag{6.7}$$

The next thing to say about this result, is it has the same structure as the Landauer result from our 1D example. As we will see, the object $\Gamma^s G\Gamma^{s'} G^\dagger$ can be interpreted as a density of states times a transmission matrix element.

A. Currents entering from a lead

The logic we are going to use is that we will look at all of the incoming eigenstates from a given lead, and ask what contribution they make to the current. As before, our system will be described by

$$H_{\mathrm{total}} = H + \sum_s (\Lambda_s + \Lambda_s^\dagger + H_s), \tag{6.8}$$

where Λ_s contains the terms which take a particle from the lead into the device. For simplicity, we can think about the case with 2 leads – generalizing to more is straightforward.

A.1. Calculating $G^<$

Before calculating the current, we will need to calculate

$$G^<(\omega) = \sum_\alpha |\alpha\rangle f_\alpha 2\pi\delta(\omega - E_\alpha)\langle\alpha| \tag{6.9}$$

where we are summing over all eigenstates of the entire system. The f_α's are the occupation numbers of the modes.

Let us consider an incoming wave from lead 1. The wavefunction will have four parts: The incoming wave $\phi^{(1)}_{\rm in}$, the reflected wave $\phi^{(1)}_{\rm out}$, the wave in the device ψ, and the transmitted wave $\phi^{(2)}_{\rm out}$. The Schrodinger equation will read

$$\begin{pmatrix} E-H & -\Lambda_1 & -\Lambda_2 \\ -\Lambda_1^\dagger & E-H_1 & 0 \\ -\Lambda_2^\dagger & 0 & E-H_2 \end{pmatrix} \begin{pmatrix} \psi \\ \phi^{(1)}_{\rm in}+\phi^{(1)}_{\rm out} \\ \phi^{(2)}_{\rm out} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}. \tag{6.10}$$

It is convenient to rewrite $\phi^{(1)} = \phi^{(1)}_{\rm in} + \phi^{(1)}_{\rm out} = \phi^{(1)}_0 + \chi^{(1)}$, where $\phi^{(1)}_0$ is an eigenstate of H_1 with eigenvalue E.

For concreteness, one can imagine a 1D lead, terminating at $x = 0$. Then:

$$\begin{aligned} \phi^{(1)}_{\rm in} &= Ae^{ikx} && (6.11)\\ \phi^{(1)}_{\rm out} &= RAe^{-ikx} && (6.12)\\ \phi^{(1)}_0 &= 2iA\sin(kx) && (6.13)\\ \chi^{(1)} &= (R+1)Ae^{-ikx}. && (6.14) \end{aligned}$$

We work with ϕ_0 rather than $\phi_{\rm in}$ primarily because it is easier to calculate ϕ_0: We just find the eigenstates of the isolated lead. [There are of course an infinite number of them, but we know how to deal with that.]

Problem 6.1.

6.1.1. Solve the second equation in Eq. (6.10) to express χ in terms of $\phi^{(1)}_0$ and ψ.

Solution 6.1.1. This is straightforward:

$$-\Lambda_1^\dagger\psi + (E-H_1)(\phi^{(1)}_0+\chi) = 0, \tag{6.15}$$

but

$$(E-H_1)\phi^{(1)}_0 = 0 \tag{6.16}$$

so

$$\chi = \frac{1}{E-H_1}\Lambda_1^\dagger\psi. \tag{6.17}$$

6.1.2. Solve the third equation in Eq. (6.10) to express $\phi^{(2)}$ in terms of ψ.

Solution 6.1.2. This one is even easier

$$\phi^{(2)} = \frac{1}{E-H_2}\Lambda_2^\dagger\psi. \tag{6.18}$$

6.1.3. Combine these results with the first equation to get an expression relating ψ to $\phi_0^{(1)}$. Write this in terms of the Greens function.

Solution 6.1.3. The substitution yields

$$\left[E - H - \Lambda_1 \frac{1}{E - H_1} \Lambda_1^\dagger - \Lambda_2 \frac{1}{E - H_2} \Lambda_2^\dagger\right] \psi = \Lambda_1 \phi_0^{(1)}. \tag{6.19}$$

or

$$\psi = G\Lambda_1 \phi_0^{(1)} \tag{6.20}$$

6.1.4. We can now calculate the density matrix

$$G^<(\omega) = \sum_\alpha |\alpha\rangle 2\pi f_\alpha \delta(\omega - E_\alpha) \langle\alpha|, \tag{6.21}$$

where $|\alpha\rangle$ is the eigenstate of the entire system with energy E_α whose occupation is f_α. Generically $G^<$ will have a contribution from bound states (which we will ignore since they do not contribute to currents) and contributions from the states incident from each lead. What is the contribution to $G^<(\omega)$ from this one mode?

Solution 6.1.4. The contribution from this one mode will be

$$(G_\psi^<)_{ij} = 2\pi f \delta(\omega - E)(G\Lambda_1 \phi_0^{(1)})_i ((\phi_0^{(1)})^* \Lambda_1^\dagger G^\dagger)_j \tag{6.22}$$

where

$$f = \frac{1}{e^{\beta_1(E-\mu_1)} + 1} \tag{6.23}$$

is the occupation of the incoming mode.
In perhaps clearer notation

$$(G_\psi^<)_{ij} = G\Lambda_1 |\phi_0\rangle 2\pi f \delta(\omega - E) \langle\phi_0| \Lambda_1^\dagger G^\dagger \tag{6.24}$$

Adding up all the contributions, the density matrix will then be

$$G^< = \sum_s f_s G \Gamma_s G^\dagger \tag{6.25}$$

$$= \sum_s G \Sigma_s^< G^\dagger \tag{6.26}$$

where

$$\Gamma_s = 2\mathrm{Im}\Sigma_s \tag{6.27}$$

$$= \Lambda_s \left(\sum_\alpha |\alpha\rangle 2\pi \delta(\omega - E_\alpha) \langle\alpha| \right) \Lambda_s^\dagger. \tag{6.28}$$

In more explicit notation

$$\begin{aligned}(\Gamma_s)_{ij} &= 2\mathrm{Im}(\Sigma_s)_{ij} && (6.29)\\ &= \sum_\alpha (\Lambda_1 \phi^{(s)}_{0,\alpha})_i 2\pi\delta(\omega - E^s_\alpha)((\phi^{(s)}_{0,\alpha})^* \Lambda_1^\dagger)_j. && (6.30)\end{aligned}$$

In the homework we have another derivation of this result, which only takes a couple lines, but is otherwise more opaque.

A.2. Current Operators

The next thing we need is an operator which yields the total current entering from a lead. A concrete place to start is with the number operator:

$$N = \sum_j a_j^\dagger a_j \tag{6.31}$$

where the sum is taken over all sites in the device. Taking a Heisenberg perspective, the total number of particles in the device obeys

$$\begin{aligned}\frac{dN}{dt} &= \frac{1}{i}[N, H_{tot}] && (6.32)\\ &= \frac{1}{i}\sum_j [a_j^\dagger a_j, H_{\mathrm{tot}}]. && (6.33)\end{aligned}$$

The only terms in the Hamiltonian that contribute are those that involve Λ and $\Lambda^\dagger$. In particular, Λ is of the form

$$\Lambda = \sum_{ij} \lambda_{ij} a_i^\dagger b_j \tag{6.34}$$

where j is in the lead, and i is in the device.

Problem 6.2.

6.2.1. Calculate $[a_j^\dagger a_j, b_s^\dagger a_t]$.

6.2.2. Calculate $[a_j^\dagger a_j, a_t^\dagger b_s]$.

6.2.3. Calculate $\frac{1}{i}[N, \Lambda + \Lambda^\dagger]$, where

$$\begin{aligned}N &= \sum_j a_j^\dagger a_j && (6.35)\\ \Lambda &= \sum_{ij} \lambda_{ij} a_i^\dagger b_j && (6.36)\end{aligned}$$

That last result can be summarized as

$$\frac{d\hat{N}}{dt} = -\sum_s \frac{\hat{\Lambda}_s - \hat{\Lambda}_s^\dagger}{i}. \tag{6.37}$$

The operators on the right hand side can be interpreted as the current operator. It acts between sites in the system and sites in the leads.

We now consider the contribution to the current from a single mode. Suppose the mode corresponds to an incoming wave from lead 1. The wavefunction in lead 1 is

$$\begin{aligned} \phi^{(1)} &= \phi_0 + \frac{1}{E - H_1}\Lambda_1^\dagger \psi & (6.38)\\ &= \phi_0 + G_1 \Lambda_1^\dagger \psi & (6.39) \end{aligned}$$

The wavefunction in lead $s \neq 1$ is

$$\begin{aligned} \phi^{(s)} &= \frac{1}{E - H_s}\Lambda_s^\dagger \psi & (6.40)\\ &= G_s \Lambda_s^\dagger \psi. & (6.41) \end{aligned}$$

The wavefunction in the device is

$$\psi = G\Lambda_1 \phi_0. \tag{6.42}$$

These can be rearranged to become

$$\begin{aligned} \Lambda_1 \phi^{(1)} &= \Lambda_1 \phi_0 + \Sigma_1 \psi & (6.43)\\ &= G^{-1}\psi + \Sigma_1 \psi & (6.44)\\ \Lambda_s \phi^{(s)} &= \Sigma_s \psi & (6.45)\\ & & (6.46) \end{aligned}$$

The contribution to the rate of change of N from this state is then

$$\begin{aligned} \frac{dN}{dt} &= -\sum_s \frac{\psi^\dagger \Lambda_s \phi^{(s)} - (\phi^{(s)})^\dagger \Lambda_s^\dagger \psi}{i} & (6.47)\\ &= -\left(\sum_s \frac{\psi^\dagger \Sigma_s \psi - \psi^\dagger \Sigma_s^\dagger \psi}{i}\right) - \frac{\psi^\dagger \Lambda_1 \phi_0 - \phi_0^\dagger \Lambda_1^\dagger \psi}{i}. & (6.48) \end{aligned}$$

It is natural to interpret the first term as the outgoing flux, and the second term as the incoming flux.

Lets first look at the incoming term. The contribution from that one mode is

$$\left(\frac{dN}{dt}\right)_{\text{in}} = -\frac{\psi^\dagger \Lambda_1 \phi_0 - \phi_0^\dagger \Lambda_1^\dagger \psi}{i} \tag{6.49}$$

$$= -\frac{\phi_0^\dagger \Lambda_1^\dagger G^\dagger \Lambda_1 \phi_0 - \phi_0^\dagger \Lambda_1^\dagger G \Lambda_1 \phi_0}{i} \tag{6.50}$$

$$= \phi_0^\dagger \Lambda_1^\dagger A \Lambda_1 \phi_0. \tag{6.51}$$

To get the total incoming current, we sum over all ϕ_0, weighting each by the probability of being occupied

$$\left(\frac{dN}{dt}\right)_{\text{total in from 1}} = \sum_\alpha f_\alpha \phi_\alpha^\dagger \Lambda_1^\dagger A \Lambda_1 \phi_\alpha \tag{6.52}$$

$$= \int \frac{d\omega}{2\pi} 2\pi \delta(\omega - E_\alpha) f_\alpha \phi_\alpha^\dagger \Lambda_1^\dagger A \Lambda_1 \phi_\alpha \tag{6.53}$$

$$= \int \frac{d\omega}{2\pi} \mathrm{Tr}\, \Sigma_1^< (\omega) A(\omega). \tag{6.54}$$

Next we look at the outgoing terms.

$$\left(\frac{dN}{dt}\right)_{\text{out}} = -\sum_s \frac{\psi^\dagger \Sigma_s \psi - \psi^\dagger \Sigma_s^\dagger \psi}{i} \tag{6.55}$$

$$= \sum_s \psi^\dagger \Gamma_s \psi, \tag{6.56}$$

which is clearly the sum of contributions leaving through each lead. Summing over all states

$$\left(\frac{dN}{dt}\right)_{\text{total out through s}} = \sum_\alpha f_\alpha \psi_\alpha^\dagger \Gamma_s \psi_\alpha \tag{6.57}$$

$$= \int \frac{d\omega}{2\pi} 2\pi \delta(\omega - E_\alpha) f_\alpha \psi_\alpha^\dagger \Gamma_s \psi_\alpha \tag{6.58}$$

$$= \int \frac{d\omega}{2\pi} \mathrm{Tr}\, G^< \Gamma_s. \tag{6.59}$$

Thus the net current through any particular lead is

$$I_s = 2q \int \frac{d\omega}{2\pi} \mathrm{Tr}\left[\Sigma_s^< A - \Gamma_s G^<\right]. \tag{6.60}$$

A.3. Linear Response

To arrive at the equation we started the lecture with, we use

$$A = \sum_s G \Gamma_s G^\dagger \tag{6.61}$$

$$G^< = \sum_s f_s G \Gamma_s G^\dagger \tag{6.62}$$

first write

$$\frac{I_s}{2q} = \int \frac{d\omega}{2\pi} \mathrm{Tr}\left[\Sigma_s^< A - \Gamma_s G^<\right] \tag{6.63}$$

$$= \int \frac{d\omega}{2\pi} \mathrm{Tr} \sum_{s'} \left[\Sigma_s^< G \Gamma_{s'} - \Gamma_s G \Sigma_{s'}^< G^\dagger\right] \tag{6.64}$$

$$= \int \frac{d\omega}{2\pi} \mathrm{Tr} \sum_{s'} \left[(f_s - f_{s'}) \Gamma_s G \Gamma_{s'} G^\dagger\right]. \tag{6.65}$$

But $f_s - f_s'$ is zero except near the Fermi surface. We can thus take everything else out of the integral, evaluating them at the Fermi energy, and arrive at

$$\frac{I_s}{2q} = \sum_{s'} \mathrm{Tr}[\Gamma_s G \Gamma_{s'} G^\dagger] \int \frac{d\omega}{2\pi} (f_s - f_{s'}) \tag{6.66}$$

$$= \sum_{s'} \mathrm{Tr}[\Gamma_s G \Gamma_{s'} G^\dagger] \frac{V_s - V_{s'}}{2\pi}, \tag{6.67}$$

which, up to a $\hbar$ that I left off somewhere, is the desired expression.

B. Currents/densities inside the device

We can calculate any single particle properties inside the devices from

$$G^< = \sum_s f_s \, G \Gamma_s G^\dagger. \tag{6.68}$$

In particular, given any single particle operator X,

$$\langle X \rangle = \int \frac{d\omega}{2\pi} \mathrm{Tr}\, G^< X. \tag{6.69}$$

In particular, if we want to calculate the deviation of $\langle X \rangle$ from its value in the absence of transport, we would calculate

$$\langle \delta X \rangle = \int \frac{d\omega}{2\pi} (f_s - f_0) \mathrm{Tr}\, G \Gamma_s G^\dagger X. \tag{6.70}$$

In linear response this is

$$\langle \delta X \rangle = \sum_s \frac{V_s}{2\pi} \mathrm{Tr}\, G \Gamma_s G^\dagger X. \tag{6.71}$$

where we evaluate the matrices at the Fermi level.

Perhaps the most useful quantity is the current. If our Hamiltonian is

$$H = \sum_{ij} H_{ij} a_i^\dagger a_j, \tag{6.72}$$

then the net current flowing between site i and j is

$$J_{ij} = \frac{2q}{\hbar}\frac{H_{ij}a_i^\dagger a_j - H_{ji}a_j^\dagger a_i}{i}, \tag{6.73}$$

where the 2 is for spin.

C. Homework

Problem 6.3. Slick (but less transparent) derivation of Density Matrix For this argument we will include the small complex shift so that

$$G = \frac{1}{\omega - H - \Sigma + i\eta}. \tag{6.74}$$

Thus

$$A = i(G - G^\dagger). \tag{6.75}$$

The energy ω will be real, H will be Hermitian, but Σ will not. In particular

$$\Gamma = i(\Sigma - \Sigma^\dagger). \tag{6.76}$$

6.3.1. Relate $G^{-1} - (G^\dagger)^{-1}$ to $\Sigma^\dagger$ and Σ.

Solution 6.3.1.

$$G^{-1} - (G^\dagger)^{-1} = \Sigma^\dagger - \Sigma. \tag{6.77}$$

6.3.2. Use that result and Eq. (6.76) to relate $G^{-1} - (G^\dagger)^{-1}$ to Γ.

Solution 6.3.2.

$$G^{-1} - (G^\dagger)^{-1} = i\Gamma. \tag{6.78}$$

6.3.3. Show that

$$G\left[G^{-1} - (G^\dagger)^{-1}\right]G^\dagger = G^\dagger - G. \tag{6.79}$$

Solution 6.3.3. This is just multiplying.

6.3.4. Combine these results to relate A to Γ, G, and $G^\dagger$. This is the central relationship which allows us to calculate the properties of this open system.

Solution 6.3.4. Equating these gives

$$A = G\Gamma G^\dagger \tag{6.80}$$

Problem 6.4. Consider a simple device consisting of a single site coupled to two leads. We will take a_0 to remove an electron from the site, $a_{j>0}$ removes

an electron from sites in the right-lead, and $a_{j<0}$ removes an electron from the left lead. We will ignore spin.

Lets take

$$\begin{aligned} H_0 &= 0 && (6.81)\\ \Lambda_L &= -\lambda a_0^\dagger a_{-1} && (6.82)\\ \Lambda_R &= -\lambda a_0^\dagger a_1 && (6.83)\\ H_L &= \sum_{j=-\infty}^{-1} -t(a_j^\dagger a_{j-1} + a_{j-1}^\dagger a_j) && (6.84)\\ H_R &= \sum_{j=1}^{\infty} -t(a_j^\dagger a_{j-+} + a_{j+1}^\dagger a_j) && (6.85)\\ & && (6.86) \end{aligned}$$

Note $t \neq \lambda$. The strength of the coupling to the leads is different from the strength of the hopping in the leads.

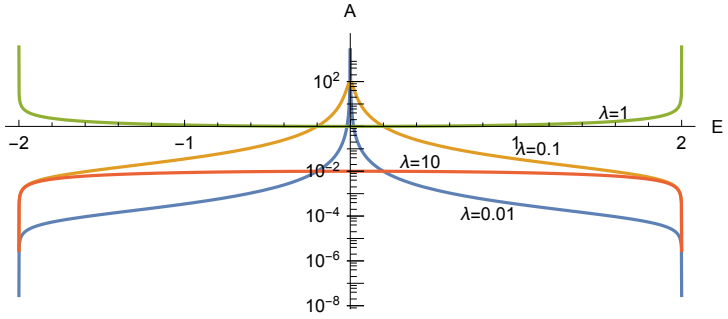
6.4.1. Find $G(\omega)$, the 1×1 matrix representing the Greens function for the single site. Feel free to use results we derived in class.

Solution 6.4.1.

$$\begin{aligned} G &= \frac{1}{E - H_0 - \Sigma_L - \Sigma_R} && (6.87)\\ &= \frac{1}{E - \frac{\lambda^2}{t}\left[\frac{E}{t} + \sqrt{\left(\frac{E}{t}\right)^2 - 4}\right]} && (6.88)\\ &= \frac{1}{\left(1 - \frac{\lambda^2}{t^2}\right)E + \frac{\lambda^2}{t}\sqrt{\left(\frac{E}{t}\right)^2 - 4}} && (6.89) \end{aligned}$$

6.4.2. Take $t = 1$. Plot the spectral density $A(\omega)$ as a function of ω for the cases $\lambda = 0.01, \lambda = 0.1, \lambda = 1, \lambda = 10$.

Solution 6.4.2. Taking just the part between $E = -2$ and $E = 2$ we have:



For $\lambda \ll 1$ this is essentially just a Lorentzian, with width $2\lambda^2$. When $\lambda \gg 1$ it crosses over to a semicircle $A \to \sqrt{4 - E^2}/\lambda^2$.

It turns out that there is also spectral weight outside of this region: For $\lambda > 1/\sqrt{2}$ the Greens function has poles at $E = \pm 2\lambda^2/\sqrt{2\lambda^2 - 1}$. These are bound states, which do not contribute to transport.

6.4.3. Assuming that the chemical potential of the left lead is $\mu_L = \mu + qV/2$ and the right lead is $\mu_R = \mu - qV/2$, find $G^<$.

Solution 6.4.3.

$$
\begin{aligned}
G^< &= G(f_L\Gamma_L + f_R\Gamma_R)G^\dagger \qquad (6.90)\\
&= \frac{\frac{\lambda^2}{2t}\sqrt{4 - \left(\frac{E}{t}\right)^2}}{\left(1 - \frac{\lambda^2}{t}\right)^2 E^2 + \left(\frac{\lambda^2}{t^2}\right)^2 \left(4 - \left(\frac{E}{t}\right)^2\right)} \left[\theta(\mu_L - E) + \theta(\mu_R - E)\right]\\
&= \frac{\frac{\lambda^2}{2t^2}\sqrt{4 - \left(\frac{E}{t}\right)^2}}{\left(1 - 2\frac{\lambda^2}{t}\right) E^2 + 4\left(\frac{\lambda^2}{t}\right)^2} \left[\theta(\mu_L - E) + \theta(\mu_R - E)\right]
\end{aligned}
$$

6.4.4. Take $\mu = 0$ and plot the current as a function of V for $\lambda = 0.1$.

Solution 6.4.4. Looks like I forgot to ask for an expression for the current before asking to plot it.
Regardless, the current from the left lead to the right lead is (setting $t = 1$)

$$J = q\int \frac{dE}{2\pi}(f_L - f_R)\Gamma_L G\Gamma_R G^\dagger \tag{6.91}$$

$$= q\int_{\mu-V/2}^{\mu+V/2} \frac{dE}{2\pi}\Gamma_L G\Gamma_R G^\dagger \tag{6.92}$$

$$= q\int_{\mu-V/2}^{\mu+V/2} \frac{dE}{2\pi}\Gamma_L^2 |G|^2. \tag{6.93}$$

We then use

$$G^2 = \frac{1}{(1-2\lambda^2)E^2 + 4\lambda^4} \tag{6.94}$$

$$\Gamma_L = \lambda^2\sqrt{4-E^2} \tag{6.95}$$

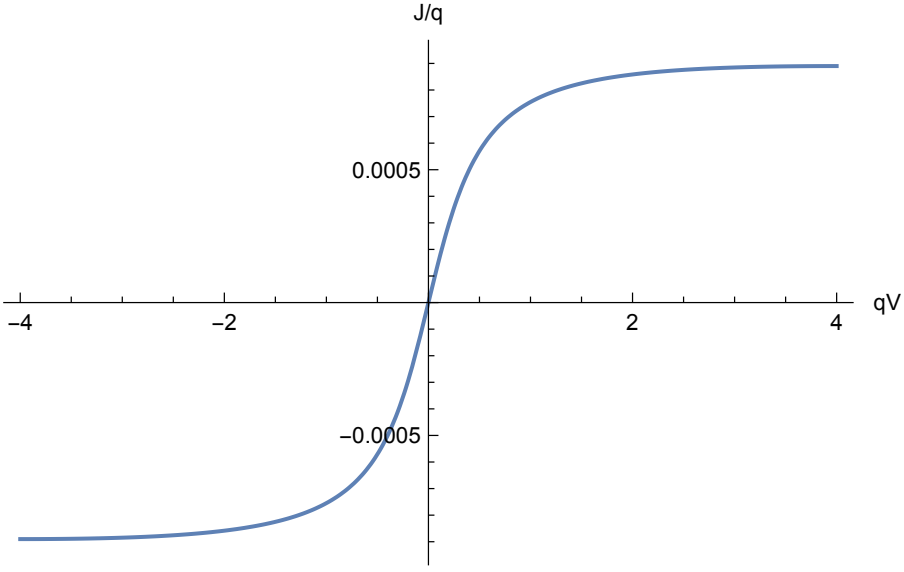
to get

$$J = q\int_{\mu-qV/2}^{\mu+qV/2} \frac{dE}{2\pi}\lambda^4 \frac{4-E^2}{(1-2\lambda^2)E^2 + 4\lambda^4} \tag{6.96}$$

Which can be done analytically. In particular, setting $\mu = 0$ we get

$$J = \frac{2}{\pi}q\lambda^3\left[\frac{1-\lambda^2}{1-2\lambda^2)^{3/2}}\arctan\left(\frac{qV\sqrt{1-2\lambda^2}}{4\lambda}\right) - \frac{qV\lambda}{4(1-2\lambda^2)}\right]. \tag{6.97}$$

Taking $\lambda = 0.1$ we get



Note that the current saturates when all the left-moving states are filled, and all of the right-moving states are empty.

6.4.5. Find an expression for the current as a function of μ and λ, in the linear response regime where V is small.

Solution 6.4.5.

$$J = \frac{q^2 V}{2\pi} \lambda^4 \frac{4-\mu^2}{\mu^2(1-2\lambda^2)+4\lambda^4} \tag{6.98}$$

When $\lambda \to 1$ this becomes the Landauer result

$$J \to \frac{q^2 V}{2\pi} \tag{6.99}$$

6.4.6. Take $V = 0, t = 1$. Find an expression for the number of particles on the dot as a function of μ and λ. This will take the form of an integral which one cannot do in closed form. [Actually that was a lie – it is an elementary integral.]

Solution 6.4.6. It turns out we can actually do the integral analytically. The expression I was originally looking for is just:

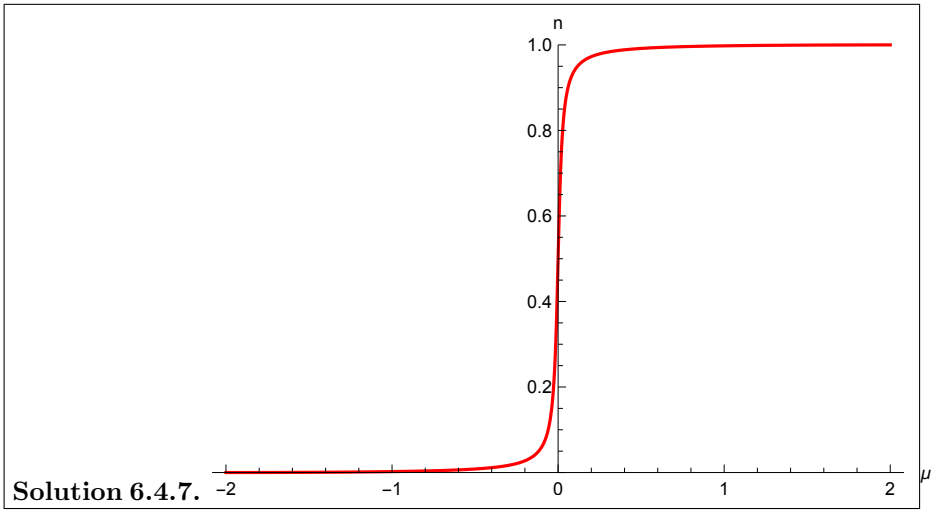
$$n = \int_{-2}^{\mu} \frac{dE}{2\pi} \frac{2\lambda^2\sqrt{4-E^2}}{(1-2\lambda^2)E+4\lambda^4}. \tag{6.100}$$

We can convert the integrand to a ratio of polynomials by the transformation $E = (z + 1/z)$. The integral can then be done by a partial fraction expansion – which gives the sum of three logs. Alternatively, you can type it into Mathematica, which gives

$$n = \frac{1}{\pi} \frac{(1-\lambda^2)\arctan\left(\frac{\mu}{\sqrt{4-\mu^2}}\frac{1-\lambda^2}{\lambda^2}\right) - \lambda^2 \arctan\left(\frac{\mu}{4-\mu^2}\right)}{1-2\lambda^2} + \frac{1}{2}. \tag{6.101}$$

This can simplify a little bit if you write it in terms of $\arcsin(\lambda)$, but I will spare you the arithmetic.

6.4.7. Plot the number of particles as a function of μ from question 6.4.6 for the case $\lambda = 0.1$.



Solution 6.4.7.

Chapter 7

Calculating Transport Using Python/Kwant

This chapter is out of sequence. I have to be out of town, and we will make it up with a computer lab. Date TBD

Chapter 8

Revisit – Feb 16, 2018

A. Concrete Example

As a concrete example, lets consider the transport through a clean 1D wire. We already know the answer to this one – we did it in lecture 1. We will, however, now approach it using greens functions. Lets take the system to be a single site, and the leads to be 1D chains extending to each side.

B. Greens functions

The Greens function for the first site of each lead is

$$G_L = G_R = \frac{1}{J}\left[\frac{E}{2J} + \sqrt{\frac{E^2}{4J^2} - 1}\right]. \tag{8.1}$$

Physically, these Greens functions tell you about the response of the lead to a perturbation where you try to tunnel in a particle at that first site. The spectral densities, which count states are

$$A_L = A_R = \frac{1}{J}\sqrt{4 - \frac{E^2}{J^2}}. \tag{8.2}$$

The Greens function for the site is

$$\begin{aligned} G &= \frac{1}{E - H_0 - \Sigma} && (8.3)\\ &= \frac{1}{E - \Sigma} && (8.4)\\ &= \frac{1}{E - J^2(G_L + G_R)} && (8.5)\\ &= \frac{-1}{\sqrt{E^2 - 4J^2}} && (8.6)\\ &= \frac{i}{\sqrt{4J^2 - E^2}} && (8.7) \end{aligned}$$

Here we used that

$$\Sigma_L = J^2 G_L. \tag{8.8}$$

Following the order of last lecture, suppose we want to know the density on the site of interest. To calculate this density we first calculate

$$G^<(E) = \sum_j f_j |\psi_j|^2 2\pi\delta(E - E_j) \tag{8.9}$$

where the sum is over all eigenstates of the entire system. The coefficient ψ_j is the amplitude that this wavefunction is on the device site. the coefficient f_j is the probability that the state is occupied.

The density is then

$$n = \int \frac{dE}{2\pi} G^<(E). \tag{8.10}$$

To calculate $G^<(E)$, we begin by noting that

$$G^{-1} - (G^\dagger)^{-1} = \Sigma^\dagger - \Sigma = i\Gamma. \tag{8.11}$$

Thus

$$G[G^{-1} - (G^\dagger)^{-1}]G^\dagger = iG\Gamma G^\dagger \tag{8.12}$$

But this expression is also

$$G[G^{-1} - (G^\dagger)^{-1}]G^\dagger = G^\dagger - G = iA. \tag{8.13}$$

Thus

$$A = G\Gamma G^\dagger. \tag{8.14}$$

The contribution to A from the states in the left lead is

$$A_{\text{fromleft}} = G\Gamma_L G^\dagger. \tag{8.15}$$

The contribution to A from the states in the right lead is

$$A_{\text{fromright}} = G\Gamma_R G^\dagger. \tag{8.16}$$

Thus the we should have

$$G^< = f_L G\Gamma_L G^\dagger + f_R G\Gamma_R G^\dagger. \tag{8.17}$$

If we take a zero-temperature model

$$\begin{aligned} G^<(E) &= \theta(\mu_L - E)\frac{i}{\sqrt{4J^2 - E^2}} J\sqrt{\frac{1}{4} - \frac{E^2}{J^2}}\frac{-i}{\sqrt{4J^2 - E^2}} && (8.18)\\ &\quad +\theta(\mu_R - E)\frac{i}{\sqrt{4J^2 - E^2}} J^2\sqrt{\frac{1}{4} - \frac{E^2}{J^2}} frac{-i}{\sqrt{4J^2 - E^2}} && (8.19)\\ &= \frac{1}{2}\left[\theta(\mu_L - E) + \theta(\mu_R - E)\right]\frac{1}{\sqrt{4J^2 - E^2}}. && (8.20) \end{aligned}$$

The number of particles is then

$$\begin{aligned} n &= \frac{1}{\pi}\left[\int_{-2J}^{\mu_L}\frac{dE}{\sqrt{4J^2 - E^2}} + \int_{-2J}^{\mu_L}\frac{dE}{\sqrt{4J^2 - E^2}}\right] && (8.21)\\ &= \frac{1}{\pi}\left[\arctan\frac{\mu_L}{\sqrt{4J^2 - \mu_L^2}} + \arctan\frac{\mu_R}{\sqrt{4J^2 - \mu_R^2}}\right]. && (8.22) \end{aligned}$$

This is just the density of particles coming from the left plus the density of particles coming from the right.

C. wavefunctinos

Last day we had an involved discussion, which started from noting that a general eigenstate incident from the left lead can be written

$$\begin{aligned} |\psi\rangle &= G\Lambda_L|\phi_0\rangle && (8.23)\\ |\phi_L\rangle &= |\phi_0\rangle + G_L\Lambda_L^\dagger|\psi\rangle && (8.24)\\ |\phi_R\rangle &= G_R\Lambda_R^\dagger|\psi\rangle. && (8.25) \end{aligned}$$

It is useful to think of how that works here. A generic state of the isolated left lead is

$$\psi_j^{(0)} = \frac{1}{\sqrt{L}}\sin(kj) \quad \text{j¡0} \tag{8.26}$$

But the dispersion is

$$E = -J\cos(k). \tag{8.27}$$

Thus

$$G \propto \frac{1}{\sin(k)} \tag{8.28}$$

is exactly the right thing to produce $1/\sqrt{L}$.

D. currents

Next we want to calculate the currents. The operator which corresponds to the current incident from the left is

$$J_L = \frac{q}{\hbar}\frac{\Lambda_L^\dagger - \Lambda_L}{i} \tag{8.29}$$

$$\Lambda_L = -Ja_0^\dagger a_{-1}. \tag{8.30}$$

Thus the total current incident from the left is

$$\langle J_L\rangle = \frac{q}{\hbar}\sum_j f_j \frac{-J(\phi_j^*\psi_j - \psi_j^*\phi_j)}{i}, \tag{8.31}$$

$$= \frac{q}{\hbar}\sum_j f_j \frac{-J((\phi_j^0)^*\psi_j - (\psi_j^0)^*\phi_j)}{i}, \tag{8.32}$$

$$+\frac{q}{\hbar}\sum_j f_j \frac{-J((\chi_j)^*\psi_j - (\chi_j)^*\phi_j)}{i},$$

where ϕ_j is the amplitude for the j'th wavefunction to be on the site -1 and ψ_j is the corresponding amplitude to be on the site 0.

We can divide this current into two parts – one corresponding to states which are incident from the left, and one corresponding to states which are incident from the right. The incident from the left has two contributions

$$\langle J_L\rangle_{\rm infromleft} = \frac{q}{\hbar}\int\frac{dE}{2\pi}f_L(E)\sum_j 2\pi\delta(E-E_j)\frac{1}{i}\left[\langle\phi_j|\Lambda_L^\dagger|\psi_j\rangle - \langle\psi_j|\Lambda_L|\phi_j\rangle\right]$$

$$= \frac{q}{\hbar}\int\frac{dE}{2\pi}f_L(E)\sum_j 2\pi\delta(E-E_j)\frac{1}{i} \tag{8.33}$$

$$\times\left[\langle\phi_j|\Lambda_L^\dagger G\Lambda_L|\phi_j\rangle - \langle\phi_j^0|\Lambda_L^\dagger G^\dagger\Lambda_L|\phi_j^0\rangle\right] \tag{8.34}$$

$$= \frac{q}{\hbar}\int\frac{dE}{2\pi}f_L(E)\sum_j 2\pi\delta(E-E_j)\langle\phi_j|\Lambda_L^\dagger A\Lambda_L|\phi\rangle \tag{8.35}$$

$$= \frac{q}{\hbar}\int\frac{dE}{2\pi}f_L(E){\rm Tr}\Sigma_L(E)A(E). \tag{8.36}$$

Where we used

$$|\psi\rangle = G\Lambda_1|\phi^0\rangle. \tag{8.37}$$

The contribution from the right is

$$\begin{aligned}\langle J_L\rangle_{\text{fromright}} &= \frac{q}{\hbar}\int\frac{dE}{2\pi}f_R(E)\sum_j 2\pi\delta(E-E_j)\frac{1}{i}\left[\langle\phi_j|\Lambda_L^\dagger|\psi_j\rangle - \langle\psi_j|\Lambda_L|\phi_j\rangle\right] \quad (8.38)\\ &= \frac{q}{\hbar}\int\frac{dE}{2\pi}f_R(E)\sum_j 2\pi\delta(E-E_j)\frac{1}{i}\left[\langle\psi_j|\Lambda_L G_L^\dagger\Lambda_L^\dagger|\psi_j\rangle - \langle\psi_j|\Lambda_L G_L\Lambda_1^\dagger|\psi_j\rangle\right]\\ &= -\frac{q}{\hbar}\int\frac{dE}{2\pi}f_R(E)\sum_j 2\pi\delta(E-E_j)\langle\psi_j|\Gamma_L|\psi_j\rangle \quad (8.39)\end{aligned}$$

where we used

$$|\phi\rangle = G_L\Lambda_L^\dagger|\psi\rangle. \quad (8.40)$$

and

$$\Gamma_L = \frac{1}{i}(\Sigma_L^\dagger - \Sigma_L) = \frac{1}{L}\Lambda_L(G_L^\dagger - G_L)\Lambda_L \quad (8.41)$$

Again this can be taken to be a trace

$$\langle J_L\rangle_{\text{fromright}} = -\frac{q}{\hbar}\int\frac{dE}{2\pi}f_R(E)\text{Tr}\Gamma_L G\Gamma_R G^\dagger \quad (8.42)$$

The backscattering contribution is the same but with R replaced by L. The net result is

$$\langle J_L\rangle = \frac{q}{\hbar}\int\frac{dE}{2\pi}(f_L(E) - f_R(E))\text{Tr}\Gamma_L G\Gamma_R G^\dagger \quad (8.43)$$

Chapter 9

Scattering

We did not get to this in class, but I wanted to briefly mention it. Inelastic scatterers can be added by a small change to our expressions. The Greens function will be

$$\sum_j (E\delta_{ij} - H_{ij} - \Sigma_{ij}(E))G_{jk}(E) = \delta_{ik}, \tag{9.1}$$

where $\Sigma(E)$ has contributions from each of the leads, and also a contribution from scatterers. The simplest model for quasi-elastic scattering would be

$$(\Sigma_{\rm scatt})_{ij}(E) = \delta_{ij} D_i G_{ii}(E), \tag{9.2}$$

where D_i encodes the strength of the scattering at site i. Similarly, we would define

$$(\Sigma_{\rm scatt})^<_{ij}(E) = \delta_{ij} D_i G^<_{ii}(E). \tag{9.3}$$

The correlation function then follows the standard expression

$$G^<(\omega) = G(\omega)\left[\Sigma_{\rm scatt})^< + \sum_s \Sigma^<_s(\omega)\right] G^\dagger(\omega). \tag{9.4}$$

Now $G^<$ appears on both sides. The equation, however, is still linear, so can be easily solved.

The current through lead s is

$$J_s = \frac{q}{\hbar}\int \frac{dE}{2\pi} {\rm Tr}\left[\Sigma^<_s(E)A(E) - \Gamma_s(E)G^<(E)\right]. \tag{9.5}$$

A. Derivation

To derive Eq. 9.2 it is convenient to first redefine the Greens functions as Fourier transforms such as

$$G(\omega) = \int d(t-t')G(t,t'). \tag{9.6}$$

We then define the two-time functions via

$$G_{ij}(t,t') = \frac{1}{i}\theta(t-t')\langle a_i(t)a_j^\dagger(t') + a_j^\dagger(t')a_i(t)\rangle \tag{9.7}$$

$$G_{ij}^<(t,t') = \langle a_j^\dagger(t')a_i(t)\rangle. \tag{9.8}$$

One can readily verify that in the case where everything is coherent, these definitions are equivalent to the ones we have previously used. To model local inelastic impurities we add a bunch of Harmonic oscillators which couple to the density on a given site, $H = H_0 + \tilde{H}$ with $\tilde{H} = \sum_j \tilde{H}_j$

$$\tilde{H}_j = \sum_q \omega_q c_q^\dagger c_q + \lambda_q(c_q^\dagger + c_q)a_j^\dagger a_j, \tag{9.9}$$

where the $c's$ and λ's differ from site to site. At this point one can work either with diagrams or equations of motion. The former is a bit more transparent, but requires a bit more background. Thus we follow the second tack.

The equations of motion for the field operators read

$$(i\partial_t - H_0)a_j - \sum_q \lambda_q(c_q^\dagger + c_q)a_j = 0, \tag{9.10}$$

which yields equations for the correlation functions

$$i\partial_t\langle a_i^\dagger(t')a_j(t)\rangle - \sum_k (H_0)_{jk}\langle a_i^\dagger(t')a_k(t)\rangle - \sum_q \lambda_q\langle a_i^\dagger(t')(c_q^\dagger(t) + c_q(t))a_j(t)\rangle = 0. \tag{9.11}$$

One then inspects the equation of motion for c_q, finding,

$$i\partial_t c_q = \omega_q c_q + \lambda_q a_j^\dagger a_j \tag{9.12}$$

$$i\partial_t c_q^\dagger = -\omega_q c_q^\dagger - \lambda_q a_j^\dagger a_j. \tag{9.13}$$

We introduce a Greens function

$$G_q(t) = \frac{1}{i}\theta(t)e^{-i\omega_q t}, \tag{9.14}$$

with Fourier transform

$$G_q(\omega) = \frac{1}{\omega - \omega_q}, \tag{9.15}$$

so that

$$c_q(t) = \lambda_q \int d\bar{t} G_q(t-\bar{t}) a_j^\dagger(\bar{t}) a_j(\bar{t}). \tag{9.16}$$

Similarly

$$c_q^\dagger(t) = \lambda_q \int d\bar{t} \bar{G}_q(t-\bar{t}) a_j^\dagger(\bar{t}) a_j(\bar{t}). \tag{9.17}$$

where

$$\bar{G}_q(t) = \frac{-1}{i}\theta(t) e^{i\omega_q t}, \tag{9.18}$$

with Fourier transform

$$\bar{G}_q(\omega) = \frac{1}{-\omega - \omega_q}. \tag{9.19}$$

To keep the notation clean, we define

$$W_q = G_q + \bar{G}_q, \tag{9.20}$$

Allowing us to write

$$\langle a_i^\dagger(t')(c_q(t) + c_q^\dagger(t) a_j(t)\rangle = \int d\bar{t} W_q(t-\bar{t}) \langle a_i^\dagger(t') a_j^\dagger(\bar{t}) a_j(\bar{t}) a_j(t)\rangle. \tag{9.21}$$

We then make a "Hartree" approximation,

$$\langle a_i^\dagger(t') a_j^\dagger(\bar{t}) a_j(\bar{t}) a_j(t)\rangle \approx \langle a_i^\dagger(t') a_j(\bar{t})\rangle \langle a_j^\dagger(\bar{t}) a_j(t)\rangle. \tag{9.22}$$

Substituting back into Eq. (9.11) yields

$$\sum_k \left[i\partial_t \langle \delta_{jk} - (H_0)_{jk} - \int d\bar{t} \Sigma_{ik}(t-\bar{t}) \langle a_i^\dagger(t') a_k(t)\rangle \right] = 0 \tag{9.23}$$

with

$$\Sigma_{ik}(t) = \delta_{ik} \sum_q \lambda_q^2 W_q(t) \langle a_i^\dagger(0) a_i(t)\rangle. \tag{9.24}$$

In Fourier space

$$\Sigma_{ik}(\omega) = \delta_{ik} \int \frac{d\nu}{2\pi} \sum_q \lambda_q^2 W_q(\nu) G_{ii}(\omega - \nu). \tag{9.25}$$

We now take the limit that the spectral density of the scatterer is sharply peaked about $\nu = 0$, to find

$$\Sigma_{ik}(\omega) = \delta_{ik} D_i G_{ii}(\omega - \nu). \tag{9.26}$$

In a diagramatic approach this amounts to summing all "rainbow" diagrams.

Mean Free Path

Our model for impurities corresponds to a mean-free time

$$\tau = \frac{1}{\Gamma} = \frac{1}{\mathrm{Im}\Sigma}. \tag{9.27}$$

This corresponds to

$$\tau = \frac{1}{D_i \rho(E)} \tag{9.28}$$

where $\rho(E)$ is the density of states.

B. Interactions

Interactions can be included by adding the appropriate self-energies. The difficulty is that generically the self-energies then become integrals over energy of products of G's. Thus Eq. (9.1) becomes a nonlinear integral equation. There is a very nice textbook by Kadanoff and Baym, which shows that in some limit this equation can be interpreted as a Boltzmann equation. I highly recommend turning there for details.