Electrons in Random Flux

MSci Project 2002

This project studies the eigenstates of an electron in a two-dimensional tightbinding model with random flux. This will involve studying the density of states (DOS) for various types of disorder. Special attention will be given to features in the DOS, such as peaks and singularities. It will also be interesting to analyse the wavefunctions of these eigenstates. This may cast light on the DOS features.

I. BASIC CONCEPTS

Impurities are unavoidable in many condensed matter systems. Although they may be a nuisance in many cases, disorder effects offer an interesting opportunity to study the physics of quantum interference.

Classical particles move diffusively when randomly scattered – imagine a ball rolling down a pin ball machine with randomly placed pins. This is the basis of the Drude theory of electrical resistance. Strong disorder leads to slower diffusion and hence a higher resistance.

In contrast, quantum particles/waves may stop diffusing altogether! This happens when their mean free path is so short that it becomes comparable to their wavelengths. Their wavefunctions become localized in space due to destructive interference. This "Anderson localization" is exhibited by electrons in dirty metals and photons in disordered dielectrics.

In this project, we will study the effect of random magnetic fields on electron motion. We will use a lattice model of electrons (tight-binding model) with random flux through each plaquette of the lattice. The eigenstates of the electrons are no longer simple plane waves. The purpose of the project is to investigate how this kind of disorder affects the density of tstates and the nature of the electron eigenstates.

A particular aspect with recent theoretical interest is the behaviour of the eigenstates near the centre of the band. Whereas the conventional theory predicets are all states are localized in two dimensions, these states appear to extend all over the system. In addition, there are appears to be a singularity in the density of states associated with this anomaly.

This project involves numerical work on the disordered system, such as the direct diagonalization of small systems and more sophisticated techniques to tackle larger systems.

You have to understand some basic concepts about electrons on a lattice. A few useful books are:

C. Kittel, Introduction to Solid State Physics G. Burns, Solid State Physics Ashcroft and Mermin, Solid State Physics

A. Tight-binding model

Instead of studying electrons in the continuum, we will use a lattice model of electron motion in solids. This is the tight-binding model. Find out about the origin and basic features of this model. Start with a one-dimensional model and then go to two dimensions.

I will also ignore the spin of the electron. In this problem, each spin state is independent of the other. Except for the exclusion principle, spin-up electrons do not see spin-down ones. So, the eigenstates and eigenenergies are not affected by spin.

Let the wavefunction have a value ψ_i at site *i*. An eigenstate with energy *E* satisfies the relation:

$$\hat{H}\psi_i = E\psi_i \tag{1}$$

where H is the Hamiltonian. For the tight-binding model,

$$\hat{H}\psi_i = -\sum_{\substack{\text{neighbours}\\j}} t_{ij}\psi_j \tag{2}$$

where the sum is over the nearest neighbours to site i on the lattice. On a square lattice, this would involve 4 neighbours.

The energy t_{ij} on each link of the lattice is called the *overlap integral*. For a homogeneous system with no disorder, all the overlap integrals are the same: $t_{ij} = t$. It is the energy scale that controls the bandwidth (see below). It is also roughly the kinetic energy cost for confining the particle to a single site (see below, eqn (4)).

We will work with *periodic boundary conditions*. By this, I mean that when an electron hops off the square lattice on the right-hand edge, it reappears on the left-hand edge, and similarly with the top and bottom edges. So, there are links between the column of sites on the right-hand edge to the column of sites on the left-hand edge. Similarly, the bottom and top edges of the lattice are joined up by links. Topologically, the system is a torus.

You should be able to show that the eigenstates are plane waves: $\psi_i = \exp(i\mathbf{k} \cdot \mathbf{r}_i)$ and that the energies of these eigenstates in a square lattice (with lattice spacing a) are:

$$E(\mathbf{k}) = -2t \left[\cos(k_x a) + \cos(k_y a)\right] \tag{3}$$

for wavevector \mathbf{k} in the first Brillouin zone. So, the bandwidth is 8t. Notice that the electrons at the bottom of the band have small wavevectors, and the dispersion relation (3) is approximately quadratic. This means that they have an effective mass m where

$$t = \hbar^2 / 2ma^2. \tag{4}$$

B. Relation to Matrices

You have probably noticed by now that, although I have written the Hamiltonian H as an operator, equation (2) is just the equation for the eigenvalues and eigenvectors of a matrix

with elements $H_{ij} = -t_{ij}$. For a system with N sites, we have an N-dimensional vector $\boldsymbol{\psi}$ and an $N \times N$ (Hermitian) matrix H_{ij} . So, the eigenvectors are the wavefunction of the electron eigenstates on the lattice. The eigenvalues are the energies of the eigenstates.

The normalisation condition for the wavefunction is just the requirement that the vector has length 1 :

$$\sum_{i} |\psi_{i}|^{2} = 1 \qquad \Leftrightarrow \qquad \psi^{\dagger} \cdot \psi = 1.$$
(5)

Sometimes, it is easier to discuss the theory of the tight-binding model as the mathematics of a matrix problem. For instance, I will often refer to the hopping integrals t_{ij} as matrix elements.

C. Density of states

The density of states (DOS) tells us about the energy spectrum of the system. For a lattice with N sites, the density of states, $\rho(E)$, is defined so that the number of eigenstates in with energy between E and $E + \delta E$ is

$$N\rho(E)\,\delta E\tag{6}$$

The factor of N is inserted to make $\rho(E)$ an intensive quantity. So, the higher $\rho(E)$ is, the more densely packed are the energies of the eigenstates around the energy E. (Think of constructing a histogram of the energies of the eigenstates, and the width of each bin is so fine that the histogram becomes a smooth function.)

Since the total number of states is the total number of sites in a tight-binding model, this means that

$$\int_{-\infty}^{\infty} \rho(E) \, dE = 1 \tag{7}$$

For the *tight-binding model*, you should be able to show from equation (3) that:

(a) the DOS approaches a constant at the band edges

$$\rho(E = \pm 4t) = \frac{1}{4\pi t a^2 \hbar^2} \tag{8}$$

(b) the DOS diverges ($\sim \ln t/E$) at the centre of the band, E = 0. (Harder) This is called a van Hove singularity.

D. Magnetic flux

In the continuum, magnetic fields affect electron motion *via* the vector potential **A**. The momentum picks up an extra bit: $\mathbf{p} \rightarrow \mathbf{p} - e\mathbf{A}$.

On a lattice, the vector potential is defined on each link of the lattice: a_{ij} for the link joining sites *i* and *j*. The tight-binding model is modified by giving the overlap integral *t* a complex phase factor: $t_{ij} \rightarrow t \exp(ia_{ij})$. The vector potential is a vector, *i.e.*, it must have a direction. If we change the direction of the link, it should change sign: $a_{ij} = -a_{ji}$.

For a square plaquette p of this lattice (with sites 1,2,3 and 4), the clockwise sum of the vector potentials gives the magnetic flux Φ_p through the plaquette:

$$\sum_{\text{plaquette}} a_{ij} = a_{12} + a_{23} + a_{34} + a_{41} = \frac{e\Phi_p}{\hbar}$$
(9)

This is the lattice analogue of $\nabla \times \mathbf{A} = \mathbf{B}$.

- (a) You should understand why a flux of Φ_m and a flux of $\Phi_p + h/e$ makes no difference to the physical behaviour of the electron.
- (b) We will be working with fluxes whose values are random from plaquette to plaquette. **Task:** Devise a scheme to calculate the vector potentials $\{a_{ij}\}$ on the links of a square lattice, given an arbitrary set of magnetic fluxes $\{\Phi_p\}$ through the plaquettes.
- (c) We will also work with periodic boundary conditions. Task: See how this affects the algorithm you proposed above. You should be led to the conclusion that the vector potentials on the links cannot be defined *unless* the total magnetic flux through the plaquettes is an integral multiple of $\Phi_0 = h/e$. (This is in fact a lattice version of the Dirac quantisation of the monopole.)

II. DISORDERED SYSTEMS

A. What do we want to know about disordered systems?

Each "sample" of our disordered lattice is defined by the set of random fluxes Φ_m through each plaquette. From this, we construct the hopping matrix elements $t_{ij} = t \exp i a_{ij}$. In principle, we can diagonalise the matrix H_{ij} and obtain all its energy eigenvalues and the corresponding eigenvectors (*i.e.* wavefunctions). However, in general, the energies and wavefunctions would be different if we used another "sample" with another set of random fluxes. So, what do we really want to know when we deal with disordered systems? The answer is that we want to know about the *statistical* properties of the eigenvalues and eigenvectors.

B. Ensemble-averaged DOS

To study statistics, we have to more precise about what we mean about random flux. I do not mean magnetic flux that is fluctuating in time. I mean static magnetic flux, but the flux is spatially random. This is called *quenched disorder*.

We will focus on the case when there is no correlation at all between the magnetic fluxes Φ_m on different plaquettes. In other words, we have N independently distributed random variables Φ_m through the N different plaquettes.

We also have to specify the probability distribution $P(\Phi)$ of the flux. We will concentrate on two cases.

- Random π -flux. $(e/h)\Phi_i = 0$ or π with equal probabilities. This gives real t_{ij} 's and real wavefunctions.
- Uniformly random flux. $(e/h)\Phi_0$ is uniformly distributed between $-\pi$ and π . This gives complex t_{ij} and the wavefunctions are complex.

This gives us properly defined "disorder ensembles".

We are concentrating on the density of the energy eigenvalues. For a particular sample, we have N eigenenergies, all between $\pm 4t$. So, the average energy difference between adjacent eigenstates is 8t/N. In principle, we can see what the density of states looks like on average by finding the energies of many samples and constructing a histogram for the energies. When we have only a few samples, say M of them, then the histogram will consist of spikes with an average separation in energy of 8t/NM. However, after we have collected the eigenenergies for many samples, we will end up with a very smooth histogram. This is the ensemble-averaged density of states we want: $\overline{\rho(E)}$ where the bar means we have averaged over the distribution for the random fluxes.

III. DOS ALGORITHM

The problem with diagonalising many samples is that the computer has to diagonalise large matrices if we want to study larger lattices — a 10×10 lattice involves a 100×100 matrix! Here is an algorithm that can generate the density of states without doing diagonalisations. The price we pay is that we do not get any wavefunctions.

A. Orthogonal polynomials

Our method will give us the ensemble-averaged DOS $\overline{\rho(E)}$ as a sum of orthogonal polynomials:

$$\overline{\rho(E=4t\epsilon)} = \frac{w(\epsilon)}{4t} \sum_{m=0}^{\infty} r_m P_m(\epsilon)$$
(10)

where $P_m(x)$ is a set of orthogonal polynomial and w(x) is the weight function that is associated with that particular set of orthogonal polynomials (see later). I have put in a factor of 4t to make the coefficients dimensionless. Orthogonal polynomials you already know about are Legendre and Laguerre (for the wavefunctions of the hydrogen atom), and Hermite polynomials (for simple harmonic oscillators). The *m*'th polynomial, $P_m(x)$, contains non-negative powers of x up to x^m . I include some properties of orthogonal polynomials in Appendix A.

We have to invert the above equation to find the coefficients r_m (m = 0, 1, 2, ...) for a given DOS. This is very similar to writing a function as a Fourier series and finding the Fourier coefficients, except that we use polynomials instead of cosines and sines. (I will specify which set of orthogonal polynomials later. In fact there are a few choices — see Appendix.)

Task: Show that

$$r_m = \frac{1}{d_m} \int_{-4t}^{4t} P_m(E/4t) \overline{\rho(E)} dE$$
(11)

(You will need to look at Appendix A.)

B. Computing the coefficients

Now, our task is reduced to computing the set of coefficients r_m 's. If we know these coefficients, we can reconstruct the DOS using equation (10).

Recall equation (2). It is more convenient to consider h = H/4t whose eigenvalues $\epsilon_{\alpha} = E_{\alpha}/4t$ are dimensionless and lie between -1 and 1. I will use matrix notation with matrix **h**. There are N eigenstates, labelled by α . For each eigenstate ϕ_{α} :

$$\mathbf{h}\boldsymbol{\phi}_{\alpha} = \epsilon_{\alpha}\boldsymbol{\phi}_{\alpha} \tag{12}$$

Any *arbitrary* wavefunction ψ can be written in terms of the eigenvectors as:

$$\boldsymbol{\psi} = \sum_{\alpha=1}^{N} c_{\alpha} \boldsymbol{\phi}_{\alpha} \tag{13}$$

Remember that the wavefunctions should be normalised (see eqn (5)). Let us also use normalised eigenstates: $\phi_{\alpha}^{\dagger} \cdot \phi_{\alpha} = 1$. If ψ represents a low-energy wavepacket, then c_{α} would be large if the corresponding eigenstate ϕ_{α} has low energy. If ψ has a lot of energy however, then the eigenstates of high energies would dominate in the series.

Now, consider the operation of h on an arbitrary wavefunction, it becomes:

$$\mathbf{h}\boldsymbol{\psi} = \sum_{\alpha=1}^{N} c_{\alpha} \epsilon_{\alpha} \boldsymbol{\phi}_{\alpha} \tag{14}$$

Convince yourself that, for any polynomial function $P(\epsilon)$:

$$P(\mathsf{h})\boldsymbol{\psi} = \sum_{\alpha=1}^{N} c_{\alpha} P(\epsilon_{\alpha}) \boldsymbol{\phi}_{\alpha}$$
(15)

So, the expectation value of P(h) is:

$$\boldsymbol{\psi}^{\dagger} P(\mathbf{h}) \boldsymbol{\psi} = \sum_{\alpha=1}^{N} |c_{\alpha}|^2 P(\epsilon_{\alpha})$$
(16)

Now, the trick is to realise that, if we average over the disorder ensemble, we would scramble up any information that distinguishes on eigenstate from another. Alternatively, we can average over all the arbitrary starting vectors $\boldsymbol{\psi}$ for a given sample, then no one coefficient c_{α} should be any different from the other. In either case, the average magnitude of the coefficients should be the same. Normalisation means that the average should come out as: $|c_{\alpha}|^2 = 1/N$. So, we get:

$$\overline{\boldsymbol{\psi}^{\dagger}P(\mathbf{h})\boldsymbol{\psi}} = \frac{1}{N}\sum_{\alpha=1}^{N}\overline{P(\epsilon_{\alpha})} \to 4t\int_{-1}^{1}P(\epsilon)\overline{\rho(4t\epsilon)}\,d\epsilon$$
(17)

The arrow indicates that I am converting the sum over eigenstates to an integral comes from the definition of the DOS, *i.e.* this is the process of turning a histogram into a smooth function by using arbitrarily fine intervals for binning. Comparing with eqn (11), we see that

$$r_m = \frac{1}{d_m} \,\overline{\psi^{\dagger} P_m(\mathbf{h})\psi} \tag{18}$$

where **h** is the matrix representation of the dimensionless Hamiltonian h = H/4t. This final equation relates r_m to a quantum expectation value, averaged over the ensemble or the choice of wavefunction. This is the central equation of our algorithm.

Task: Use the recursion relations (A2) to devise an efficient computational scheme to calculate r_m using equation (18).

APPENDIX A: ORTHOGONAL POLYNOMIALS

Each set of orthogonal polynomials has a domain in a < x < b where it is defined. Also, a weight function w(x) is associated with each set of polynomials so that there is an orthogonality theorem:

$$\int_{a}^{b} w(x)P_{m}(x)P_{n}(x) dE = d_{n}\delta_{m,n}$$
(A1)

where $\delta_{m,n}$ is the Kronecker delta (equal to one if m = n, otherwise it is zero.) The appearance of d_n is just a matter of convention for how to normalise the function. We can always multiply each P_n by $d_n^{1/2}$ to absorb it.

From the above definitions, it can be shown that there is a recursion relation relating consecutive polynomials:

$$P_{n+1}(x) = (a_n + b_n x) P_n(x) - c_n P_{n-1}(x)$$
(A2)

starting with $P_0(x) = 1$.

We are interested in polynomials defined in a finite range because our model has definite band edges. We can scale the energy to -1 < x < 1. Here are some examples:

Polynomial	weight $w(x)$	Convention	a_n	b_n	c_n	d_n
Legendre $P_n(x)$	1	$P_n(1) = 1$ $P_0(x) = 1, P_1(x) = x$	0	$2 - \frac{1}{n+1}$	$1 - \frac{1}{n+1}$	$\frac{2}{2n+1}$
Chebyshev 1st: $T_n(x)$	$(1-x^2)^{-1/2}$	$T_n(1) = 1$ $T_0(x) = 1, T_1(x) = x$	0	2	1	$\pi/2 \text{ for } n \neq 0$ $\pi \text{ for } n = 0$
Chebyshev 2nd: $U_n(x)$	$(1-x^2)^{1/2}$	$U_n(1) = n + 1$ $U_0(x) = 1, U_1(x) = 2x$	0	2	1	$\pi/2$

These polynomials are even functions of x for even n and odd functions for odd n.

The Chebyshev polynomials are closely related to trigonometric functions. We are using them to represent functions (see eqn (10)). This makes the link to Fourier series more than just an analogy:

$$T_n(\cos\theta) = \cos(n\theta)$$
 , $U_n(\cos\theta) = \frac{\sin[(n+1)\theta]}{\sin\theta}$ (A3)