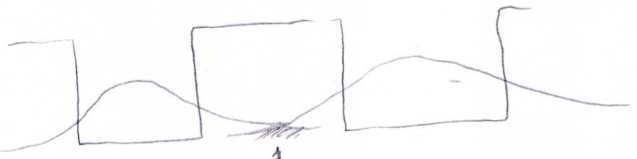
The tight-binding model

The electrons in carbon based materials (like graphene) or in semiconductors, are not free to move like in metals. Instead, they spend most of their lives sitting on atomic sites. But every once in a while, due to a small overlap in atomic orbitals, the electrons may tunnel from one site to another.



overlap (this drawing is terrible!)

This is how an electron in your phone moves: it hops from one site to another. Tight-binding is the generic name we give to models of electrons hopping through a lattice. These models are widely used to understand the electronic properties of organic molecules, graphene and semiconductors.

Most scientific papers use 2nd quantization to describe the tight-binding model. This, as we will learn, has some nice advantages. But it is not a necessity. Here we will describe the model using the usual rules of QM. Later we will revisit it in 2nd quantized notation. I think that comparing the two approaches will help make the physics clearer.

The Eq numbers in the next page start on (8).
Sorry about that

Tight-binding in one dimension

Imagine that you have a 1D lattice with N sites and lattice spacing a

we label each site by $n = 1, \ldots, N$ and we choose a reference frame such that the position of each site is

$$x_n = a n \tag{8}$$

Now imagine you have an electron hopping from one site to another. It spends most of its time sitting in some lattice site but, every once in a while, it has a small probability amplitude for jumping to a neighboring site. We assume only nearest neighbor hopping since second nearest neighbor should be much less likely.

This problem can be described quantum mechanically as follows. Let $|n\rangle$ denote the state representing "the electron at site n." then the only non-zero matrix elements of the Hamiltonian will be

$$\langle n|H|n+1\rangle = \langle n+1|H|n\rangle = -\vartheta \tag{9}$$

where ϑ is the hopping amplitude and the minus sign is placed only for aesthetic reasons.

we may now introduce 2 completeness relations and write

$$H = \sum_{n,m} |n\rangle\langle n| H |m\rangle\langle m|$$

$$= \sum_{n} \left\{ |n\rangle\langle n|H|n+1\rangle\langle n+1| + |n+1\rangle\langle n+1|H|n\rangle\langle n| \right\}$$

thus H may be written as

$$H = -g \sum_{n} \left[|n+1\rangle\langle n| + |n\rangle\langle n+1| \right] \tag{10}$$

If you want, you could also write H as a big matrix. For instance, if $N = 5$ we would get

$$H = \begin{pmatrix} 0 & -g & 0 & 0 & -g \\ -g & 0 & -g & 0 & 0 \\ 0 & -g & 0 & -g & 0 \\ 0 & 0 & -g & 0 & -g \\ -g & 0 & 0 & -g & 0 \end{pmatrix} \tag{11}$$

Note the two lonely terms in the corners. They represent the periodic boundary conditions, meaning an electron at 1 can hop either to 2 or to N. this term is usually left implicit in Eq (10) by assuming that $|N+1\rangle = |N\rangle$.

writting H as a matrix, however, is not recommended. We are interested in arbitrarily large N and, very soon, we will generalize this to an arbitrary lattice in arbitrary dimension. the outer product notation (10), albeit more abstract, is much more robust.