Lecture 1: simple models of atomic insulators

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I. INTRODUCTION

I will split the course into two broad chapters. In the first part we will study insulating phases of matter while in the second part we will study metallic phases. Metals conduct electricity while insulators do not. The distinction is sharp at temperature $T = 0K$, *i.e*, at $T = 0$, insulators and metals are sharply distinct phases and there needs to be a phase transition to go from one to the other.

Let us recall that a very powerful and useful way to partially distinguish different phases of matter is to look for broken symmetries, *i.e*, symmetries of the Hamiltonian that are not symmetries of the ground (or the equillibrium state if we are interested in $T \neq 0$) state. A familiar example is the distinction between a crystalline solid and a liquid. The solid spontaneously breaks the continuous translation symmetry of atoms in space while liquids do not. This leads to a sharp distinction between the solid and the liquid. Another familiar example is in ferromagnet which spontaneously breaks the global symmetry of rotations of the spins of the underlying electrons. In contrast in a paramagnet the spin rotation symmetry is present, and hence there is a sharp distinction with the ferromagnet. The extent to which a symmetry is broken in a phase of matter is quantified by the concept of the Landau order parameter. For example, in a ferromagnet the order parameter is the spontaneous magnetization.

Note however that the distinction between a metal and an insulator is not tied to any symmetry change (or onset of any broken symmetry Landau order parameter). Indeed through out the course we will see many examples of distinctions between phases of matter that are not captured by the conventional notion of a Landau order parameter.

Insulators are simpler to treat theoretically, and so we start the discussion with them. There are many different kinds of insulators. The most familiar (from basic solid state physics) is a band insulator. These may be further subdivided into atomic insulators and topological insulators. A different kind of insulator is obtained when the electrons are localized in real space by impurities

in the solid. These are known as Anderson insulators. Finally there are insulators driven by the dominating influence of the electron-electron Coulomb interaction; these are known as Mott insulators (or slightly more generally as correlated insulators). We will not have the time to discuss Anderson insulators in this course.

II. ATOMIC INSULATORS

Consider starting with atoms with a filled shell of electrons, and putting them together to form a solid. The resulting solid will in many circumstances form an insulator. We will describe some simple models for such an insulator below.

Let us start with a trivial model for such an atomic insulator, Consider an atom with a single "ground" energy level with energy ϵ_0. (In a real atom, there will be other excited states. We assume that these have such high energy that they can be ignored, and hence not include them in our model). Assume $N\rangle\infty$ such atoms are arranged in some lattice. Further assume that each such atom has 2 electrons which therefore fill the ground energy level. In the full crystal, each of the atoms will of course continue to have their ground energy level fully occupied. Let us denote by $c^\dagger_{i\alpha}$ the electron creation operator (with $\alpha =\uparrow,\downarrow$ a spin label) for the ith atom. Clearly the many body ground state is

$$|psi_{gd}\rangle = \prod_i c^\dagger_{i\uparrow} c^\dagger_{i\downarrow}|0\rangle \tag{1}$$

Consider a Hamiltonian for this system which allows electrons to hop on or off an atom, *i.e*

$$\mathcal{H} = -\sum_{ij} t_{ij} c^\dagger_{i\alpha} c_{j\alpha} + \epsilon_0 \sum_{i\alpha} c^\dagger_{i\alpha} c_{i\alpha} \tag{2}$$

However though $\mathcal{H}$ allows electrons to move in the lattice, such motion is impossible in the state $|\psi_{gd}\rangle$ due to Pauli exclusion. Thus $\psi_{gd}\rangle$ describes an electrical insulator. Further if we fix the total number of electrons $N_e = 2N$, then there is exactly a single *many body* state in the Hilbert space (which is the state $|\psi_{gd}\rangle$). Clearly this state has no response to any external probe that does not change the electron number. In particular there is no response to an external electriic field, and we get an insulator.

We can also discuss this in (crystal) momentum space. Define the lattice Fourier transform

$$c_{i\alpha} = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}} c_{\mathbf{k}\alpha} \tag{3}$$

with $\mathbf{k} \in$ the first Brillouin zone of the crystal. Then the Hamiltonian becomes

$$\mathcal{H} = \sum_{\mathbf{k},\alpha} \epsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\alpha} c_{\mathbf{k}\alpha} \tag{4}$$

where the 'dispersion' $\epsilon_{\mathbf{k}} = -2t \sum_{\nu=1}^{d} (\cos(k_\nu a)) + \epsilon_0$, and we have for simplicity assumed a d-dimensional cubic lattice with lattice spacing a.

In the many body ground state, all the k-points are fully occupied and we get a band insulator.

Let us now generalize the model slightly and allow each atom to have multiple energy levels ϵ_n. We also allow electrons to hop between neighboring atoms. To keep things simple, to begin with, let us further assume that an electron in state n at site i can only hop to state n at a neighboring site j. The Hamiltonian then takes the form

$$\mathcal{H} = \sum_{in\alpha} \epsilon_n c^{\dagger}_{in\alpha} - \sum_{\langle ij \rangle} \sum_{n\alpha} t_n c^{\dagger}_{ni\alpha} c_{ni\alpha} \tag{5}$$

We can diagonalize this, as before, by going to the crystal momentum basis to find

$$\mathcal{H} = \sum_{n\mathbf{k}\alpha} E_n(\mathbf{k}) c^{\dagger}_{n\mathbf{k}\alpha} c_{n\mathbf{k}\alpha} \tag{6}$$

with

$$E_n(\mathbf{k}) = -2t_n \sum_{\nu=1}^{d} (\cos(k_\nu a)) + \epsilon_n \tag{7}$$

Each level now forms a band with

$$\epsilon_n - 2|t_n|d \leq E_n(\mathbf{k}) \leq \epsilon_n + 2|t_n|d \tag{8}$$

The band width of the n'th band is $W_n = 4|t_n|d$. For small $t_n| \ll \epsilon_n - \epsilon_{n'}$, distinct bands do not overlap in energy. Now suppose that each atom has n_0 filled levels, *i.e*, the number of electrons per atom is $2n_0$. Then, in the solid, n_0 bands will be fully filled and we get a band insulator.

Clearly we can generalize this model further to allow hopping between different states m, n at neighboring sites, *i.e*, the Hamiltonian

$$\mathcal{H} = \sum_{in\alpha} \epsilon_n c^{\dagger}_{in\alpha} - \sum_{\langle ij \rangle} \sum_{nm\alpha} t_{nm} c^{\dagger}_{ni\alpha} c_{mi\alpha} \tag{9}$$

In $\mathbf{k}$-space, we then have

$$\mathcal{H} = \sum_{nm\mathbf{k}\alpha} \left(\epsilon_n(\mathbf{k})\delta_{mn} - t_{nm}(\mathbf{k})\right) c^{\dagger}_{n\mathbf{k}\alpha} c_{m\mathbf{k}\alpha} \tag{10}$$

with $t_{nm}(\mathbf{k}) = 2t_{nm}\sum_{\nu=1}^{d}(\cos(k_\nu a))$. The transformation to $\mathbf{k}$-space has block diagonalized the Hamiltonian. We still need to diagonalize it in the n, m-'orbital' space. To that end, we diagonalize the matrix $T_{nm}(\mathbf{k}) = \epsilon_n(\mathbf{k})\delta_{mn} - t_{nm}(\mathbf{k})$ by solving the eigenvalue equation

$$T_{nm}(\mathbf{k})\chi_m^I(\mathbf{k}) = E^I(\mathbf{k})\chi_n^I(\mathbf{k}) \tag{11}$$

The $E^I(\mathbf{k})$ are the band dispersions of the I'th band, and so long as an integer number n_0 of bands are fully filled we get a band insulator. For small $|t_{nm}|$, we can think in real space by starting with atoms with filled shells. As $|t_{nm}|$ increases, so long as we do not encounter any phase transitions, we get qualitatively the same kind of insulating ground state.