



Keble College - Hilary 2012  
Section VI: Condensed matter physics  
Notes: Holes

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While the concept of a hole is relatively straightforward, a mathematical description of holes is complicated by competing conventions with subtle sign differences. Here, I present three self-consistent ways of looking at electrons (or holes).

## Description in terms of electrons only

### Bloch electrons

Let's consider independent electrons in a periodic potential. In this case the single electron eigenstates (Bloch eigenstates) are labelled by both a wavevector  $\mathbf{k}$ , uniquely defined up to the addition of reciprocal lattice vector, and a band index  $n$ .

We write the energy, crystal momentum and mean velocity of a Bloch eigenstate with wavevector  $\mathbf{k}$  and band index  $n$  as  $\epsilon_n(\mathbf{k})$ ,  $\tilde{\mathbf{p}} = \hbar\mathbf{k}$  and  $\mathbf{v}_n(\mathbf{k})$ . We will be concerned with other quantities that depend on these, namely the mean momentum and mean current,  $\mathbf{p}_n(\mathbf{k}) = m_e\mathbf{v}_n(\mathbf{k})$  and  $\mathbf{I}_n(\mathbf{k}) = -e\mathbf{v}_n(\mathbf{k})$ .

In thermal equilibrium at temperature  $T = 1/k_B\beta$  the occupation of single electron states with energy  $\epsilon$  is given by Fermi occupation function

$$n_F(\epsilon - \mu) = \frac{1}{e^{\beta(\epsilon - \mu)} + 1}, \quad (1)$$

with the chemical potential  $\mu$  is such that it gives the correct value for the total number of electrons.

For a full band, the total mean momentum, crystal momentum and mean current are zero.

### Semi-classical model

Working within the semi-classical model (looking at a single band and dropping the band index to simplify notation), the velocity of an electron in the single electron eigenstate labelled wavevector  $\mathbf{k}$  is given by

$$\mathbf{v}(\mathbf{k}) = \frac{1}{\hbar}\nabla_{\mathbf{k}}\epsilon(\mathbf{k}). \quad (2)$$

Further, when an electric field is applied, the wavevector  $\mathbf{k}$  of an electron evolves according to

$$\hbar\dot{\mathbf{k}} = \mathbf{F}, \quad (3)$$

where the force is given by  $\mathbf{F} = -e\mathbf{E}$ .

At a band edge, we may neglect all terms greater than quadratic in the Taylor expansion of  $\epsilon(\mathbf{k})$  around some band head  $\mathbf{k}'$ . By substitution, the velocity in this limit obeys an equation similar to Newton's second law

$$\mathbf{m}^{*-1}\mathbf{F} = \dot{\mathbf{v}}. \quad (4)$$

The inverse effective mass tensor  $\mathbf{m}^{*-1}$  can be written in matrix form in the Cartesian basis as

$$\mathbf{m}^{*-1} = \frac{1}{\hbar^2} \begin{pmatrix} \frac{\partial^2 \epsilon}{\partial k_x^2}(\mathbf{k}') & 0 & 0 \\ 0 & \frac{\partial^2 \epsilon}{\partial k_y^2}(\mathbf{k}') & 0 \\ 0 & 0 & \frac{\partial^2 \epsilon}{\partial k_z^2}(\mathbf{k}') \end{pmatrix}. \quad (5)$$

You will only ever have to worry about the one-dimensional case, e.g. along the  $x$ -axis, where this simplifies to

$$F = m^* \dot{v}, \quad (6)$$

with force  $F = -eE$  and effective mass  $m^* = \hbar^2 \left( \frac{\partial^2 \epsilon}{\partial k_x^2}(k') \right)^{-1}$ .

The above is a good way of describing a band that is only occupied by a few electrons, and in particular, only a few states near the band edge are occupied. However, it is pretty useless at describing a band that is nearly full. Trying to sum up the contributions to the momentum and current from all electrons would be difficult, and we have also made an assumption that only a few of the states near the band edge are occupied.

To describe nearly full bands, where the unoccupied states are those near a band edge, we will find it easier to focus on the absence of electrons. There are two ways of doing this (and probably others), both consistent within themselves but frustratingly different.

## Description in terms of unoccupied electron states

The first approach is used in some textbooks, including Ashcroft and Mermin. Since the mean momentum, crystal momentum and mean current of a full band is zero the mean momentum, crystal momentum and mean current of this band will be the negative sum of the the momentum, crystal momentum and current of the unoccupied single electron states. So we firstly need to find the unoccupied electron states. Then we just keep track of how the momenta and crystal momenta of these evolve, which will be given by the equations in the previous section. Finally, the contribution to the momentum, crystal momentum and current is just negative sum of what these would give.

So, as you can see, this approach is very simple, and it is useful to check that other descriptions of holes makes sense. However, it's not really fully embraced the concept of a hole, rather just dealing directly with electrons and their absences.

## Description in terms of holes

The second approach is used by the lecturer. It goes much further than the previous approach and properly introduces a particle called a hole. All physical properties of the band can then be determined from which hole states are occupied, without reference to electrons. The equivalence of the hole and electron pictures is ensured by correctly defining the properties of the hole states.

Again in what follows we focus here on a single band and drop the band index to simplify notation. We begin by defining an ideal model for holes, in analogy with that for electrons. Then we show how the free parameters of this model can be chosen such that the model gives exactly the same expectation values of physical quantities as the electron description.

### The independent hole model

The aim of this approach is to introduce holes such that their definition, occupation and evolution obey very similar equations to the electrons. So, in analogy with electrons, we would like single hole eigenstates labelled by wavevectors  $\mathbf{k}_h$ , with eigenenergies  $\epsilon_h(\mathbf{k}_h)$  and crystal momenta  $\tilde{\mathbf{p}}_h = \hbar \mathbf{k}_h$ . Similar to before we write the mean velocity of a hole state with wavevector  $\mathbf{k}_h$  as  $\mathbf{v}_h(\mathbf{k})$ , and the mean momentum and current of this hole state is  $\mathbf{p}_h = m_h \mathbf{v}_h$  and  $\mathbf{I}_h = q_h \mathbf{v}_h$ .

In thermal equilibrium at temperature  $T = 1/k_B \beta$ , a chemical potential  $\mu_h$  for the holes should determine the occupation  $n_F(\epsilon_h - \mu_h)$  of hole sates of energy  $\epsilon_h$ . This implies that we will be looking for a description where holes are fermions.

Finally, in the semiclassical model, just like we did for electrons we would like to be able to write the mean velocity of a hole in the state labelled by  $\mathbf{k}_h$  as

$$\mathbf{v}_h(\mathbf{k}_h) = \frac{1}{\hbar} \nabla_{\mathbf{k}_h} \epsilon_h(\mathbf{k}_h), \quad (7)$$

and the response to an electric field captured by

$$\hbar \dot{\mathbf{k}}_h = \mathbf{F}_h, \quad (8)$$

where the force is  $\mathbf{F}_h = q_h \mathbf{E}$ .

It follows that if there is a band head for the hole eigenstates at some wavevector  $\mathbf{k}'_h$  then near this wavevector, we have

$$\mathbf{m}^{*-1}_h \mathbf{F}_h = \dot{\mathbf{v}}_h, \quad (9)$$

where the inverse effective mass tensor  $\mathbf{m}^{*-1}_h$ , written as a matrix in the Cartesian basis is

$$\frac{1}{\hbar^2} \begin{pmatrix} \frac{\partial^2 \epsilon_h}{\partial k_{h,x}^2}(\mathbf{k}'_h) & 0 & 0 \\ 0 & \frac{\partial^2 \epsilon_h}{\partial k_{h,y}^2}(\mathbf{k}'_h) & 0 \\ 0 & 0 & \frac{\partial^2 \epsilon_h}{\partial k_{h,z}^2}(\mathbf{k}'_h) \end{pmatrix}. \quad (10)$$

In one dimension, along the  $x$ -axis, this simplifies to

$$F_h = m_h^* \dot{v}_h, \quad (11)$$

with force  $F_h = q_h E$  and effective mass  $m_h^* = \hbar^2 \left( \frac{\partial^2 \epsilon_h}{\partial k_{h,x}^2}(k') \right)^{-1}$ .

### Hole properties (in terms of electron properties)

The next stage is to impose the condition that the description in terms of holes should be physically equivalent (predict the same momentum, crystal momentum and current) to the description in terms of electrons. Then from this we can obtain expressions for  $\mathbf{k}_h$ ,  $\epsilon_h(\mathbf{k}_h)$ ,  $\mu_h$ ,  $m_h$  and  $q_h$  in terms of  $\mathbf{k}$ ,  $\epsilon(\mathbf{k})$ ,  $\mu$ ,  $m$  and  $q = -e$ . Here I will present the correct expressions and check they do indeed result in a physical equivalence between the hole and electron pictures.

We start by desiring the absence of an electron occupying state  $\mathbf{k}$  is equivalent to a hole occupying state  $\mathbf{k}_h$ . For these two pictures to predict the same energy and momentum,

$$\mathbf{k}_h = -\mathbf{k}, \quad (12)$$

$$\epsilon_h(\mathbf{k}_h) = -\epsilon(\mathbf{k}). \quad (13)$$

This also implies  $\tilde{\mathbf{p}}_h = -\tilde{\mathbf{p}}$  for the crystal momentum. To ensure that  $\mathbf{p}_h = -\mathbf{p}$  and  $\mathbf{I}_h = -\mathbf{I}$  we require

$$m_h = -m_e, \quad (14)$$

$$q_h = e. \quad (15)$$

To ensure that, at thermal equilibrium, the occupation of the hole states is exactly unity minus the occupation of the associated electron states, we have that

$$\mu_h = -\mu, \quad (16)$$

which results in the correct occupation due to the property  $n_F(\epsilon - \mu) = 1 - n_F(\mu - \epsilon)$ . One can check that Eqs. 8-11 are consistent with the above properties, with  $\mathbf{m}_h^{*-1} = -\mathbf{m}^{*-1}$  and  $m_h^* = -m_e^*$ .

### Summary of hole model

So, what this is telling us, is that we are able to take a band of electron states, and define a set of hole states, which have wavevectors in the opposite direction and the negative of the energy. Then attributing a negative mass and opposite charge to these holes, as well as defining their chemical

potential to be the negative as that for electrons<sup>1</sup> we recover exactly the same properties and identical equations as if we had instead dealt with electrons.

For each band we choose whether to talk about holes or electrons. As is the only sensible choice, for semiconductors we choose to describe the conduction band in terms of electrons and the valence band in terms of holes. This is because only electron and hole states near band edges will be occupied, ensuring the validity of the near-band-edge approximations used above description.

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<sup>1</sup>This makes physical sense if you remember one definition of the chemical potential as being the energy required to add a particle.