# Dynamics of electrons in a lattice

Notes, FYS-208, 1995 - L. Kocbach, Univ. Bergen

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In most of the textbooks on Solid State Physics this subject is treated in a so called semi-classical approximation. It is my impression that though the usual treatment gives a correct result, it is not really understandable, and in some cases even contains some wrong elements.

In this note we propose an alternative way to justify the well known result, and we also bring a few further illustrations of the concept of the effective mass. This approach has now been applied in three courses and it seems to be well understood by the students.

## Group velocity for Bloch electrons

We start from the equation for the periodic function $u_{\epsilon,\vec{k}}(\vec{x})$

$$\left[-\frac{\hbar^2}{2m}\left(\nabla + i\vec{k}\right)^2 + U(r)\right] u_{\epsilon,\vec{k}} = \epsilon(k)\ u_{\epsilon,\vec{k}} \qquad \textit{take} \qquad \frac{\partial}{\partial k_x}$$

$$\frac{\partial}{\partial k_x}\left(\nabla + i\vec{k}\right)^2 \rightarrow 2\ i\left(\nabla + i\vec{k}\right)$$

$$-\frac{\hbar^2}{m} i\left(\nabla + i\vec{k}\right) \rightarrow \frac{\hbar}{m}\left(-i\hbar\frac{\partial}{\partial x} + \hbar k_x\right)$$

This was only the part corresponding to the [.....] part. Taking the whole $k_x$-derivative and multiplying by $u^*_{\epsilon,\vec{k}}$ and integrating, we get

$$\frac{\hbar}{m}\int u^*_{\epsilon,\vec{k}}\left(-i\hbar\frac{\partial}{\partial x} + \hbar k_x\right) u_{\epsilon,\vec{k}} + \int u^*_{\epsilon,\vec{k}} H\left(\frac{\partial u_{\epsilon,\vec{k}}}{\partial k_x}\right) \;=\; \int u^*_{\epsilon,\vec{k}}\left(\frac{\partial\epsilon(k)}{\partial k_x}\right) u_{\epsilon,\vec{k}} + \int \epsilon(k) u^*_{\epsilon,\vec{k}}\left(\frac{\partial u_{\epsilon,\vec{k}}}{\partial k_x}\right)$$

We combine the second terms on each side, they give

$$\int\left\{u^*_{\epsilon,\vec{k}}\left(H - \epsilon(k)\right)\right\}\left(\frac{\partial u_{\epsilon,\vec{k}}}{\partial k_x}\right)$$

The term in the {.....} is zero ( Complex Conjugation ) We are then left with

$$\frac{\hbar}{m}\int u^*_{\epsilon,\vec{k}}\left(-i\hbar\frac{\partial}{\partial x} + \hbar k_x\right) u_{\epsilon,\vec{k}} \;= \int u^*_{\epsilon,\vec{k}}\left(\frac{\partial\epsilon(k)}{\partial k_x}\right) u_{\epsilon,\vec{k}}$$

or simply

$$\frac{\hbar}{m}\int u^*_{\epsilon,\vec{k}}\left(-i\hbar\frac{\partial}{\partial x} + \hbar k_x\right) u_{\epsilon,\vec{k}} \;= \left(\frac{\partial\epsilon(k)}{\partial k_x}\right)$$

This gives, going back to the whole wavefunctions $\psi_{\epsilon,\vec{k}}$

$$\frac{\hbar}{m}\int \psi^*_{\epsilon,\vec{k}}\left(-i\hbar\frac{\partial}{\partial x}\right)\psi_{\epsilon,\vec{k}} = \frac{\partial\epsilon(k)}{\partial k_x}$$

i.e. we can write that

$$\frac{1}{\hbar}\frac{\partial\epsilon(k)}{\partial k_x} = \frac{1}{m}\langle p_x\rangle \rightarrow \langle v_x\rangle$$

i.e. the group velocity, meaning the average velocity. Note that we have derived this by manipulations with symbols, instead of refering directly to group velocity argument.

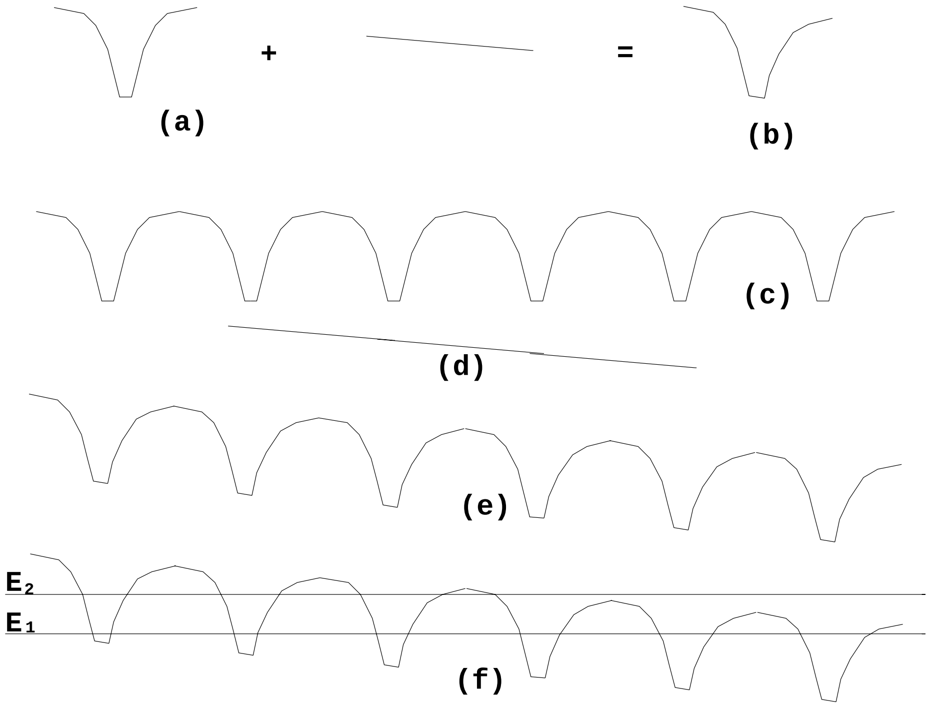

Figure 1: Potentials: Periodic plus constant field

## Bloch electrons and constant field potential

$$V(\vec{x}) = -\vec{F}.\vec{x}$$

The picture must be discussed in detai: what do the inclined bands mean.

$$\Delta\epsilon(x) \quad = \quad -\Delta V(x)$$

$E$ being the energy of a state, or central energy or a wave packet, it will correspond to different $\epsilon$ at the varying positions. It is easy to see that

$$\Delta\epsilon \;=\; -\;\Delta V$$

Since the relation between $\epsilon$ and $k$ is identical in each of the segments, we can e.g. write for each position $x$

$$\epsilon_k(x) = \epsilon(k(x))$$

where the function $\epsilon(k)$ is the relation between energy and wavenumber for force-free case. For a given wavepacket, we can write $\Delta x = v_g(x)\Delta t$, where we already indicate that even the group velocity can - and will - depend on the position.
We can thus write

$$\frac{\Delta k}{\Delta x} \rightarrow \frac{\Delta k}{v_g(x)\Delta t}$$

Once we have established this, we can go to a limiting chain

$$\frac{dk}{dt} = v_g(x)\frac{dk}{dx} = \frac{1}{\hbar}\frac{d\epsilon}{dk}\frac{dk}{dx}$$

This can be continued by realizing that $\Delta\epsilon \;=\; -\;\Delta V$,

$$\frac{dk}{dt} = \frac{1}{\hbar}\frac{d\epsilon}{dx} = -\frac{1}{\hbar}\frac{dV}{dx}$$

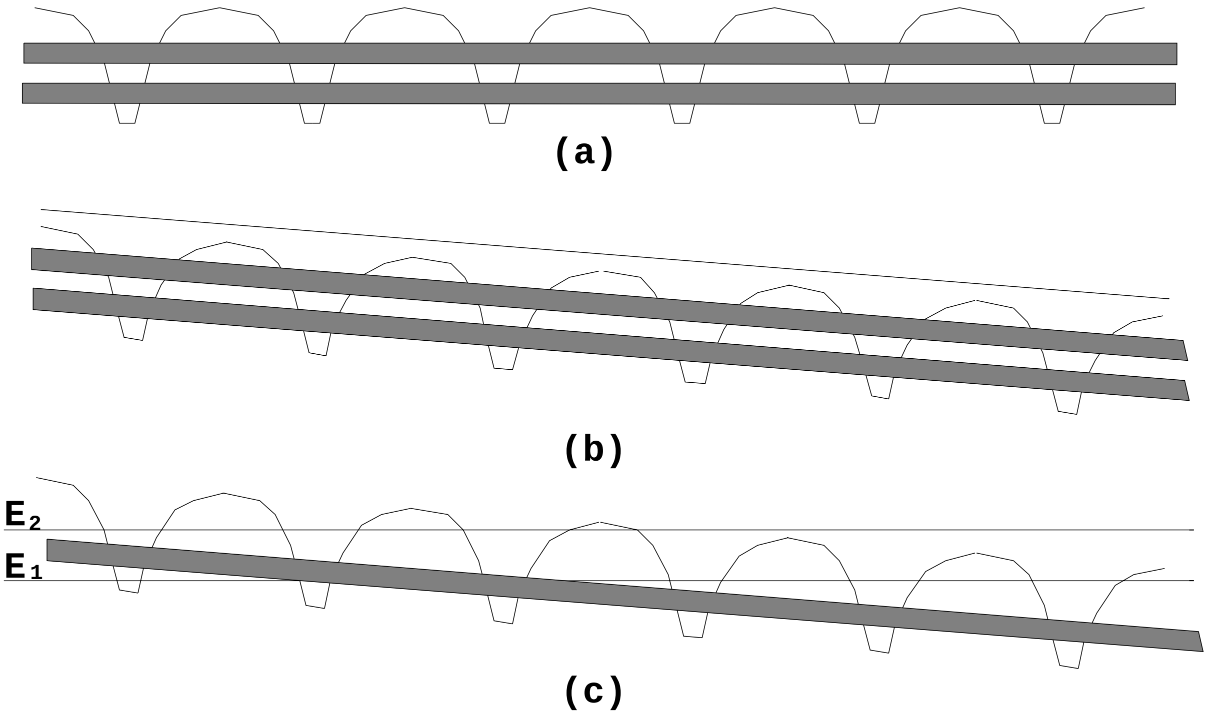

Figure 2: Bands in inclined potentials

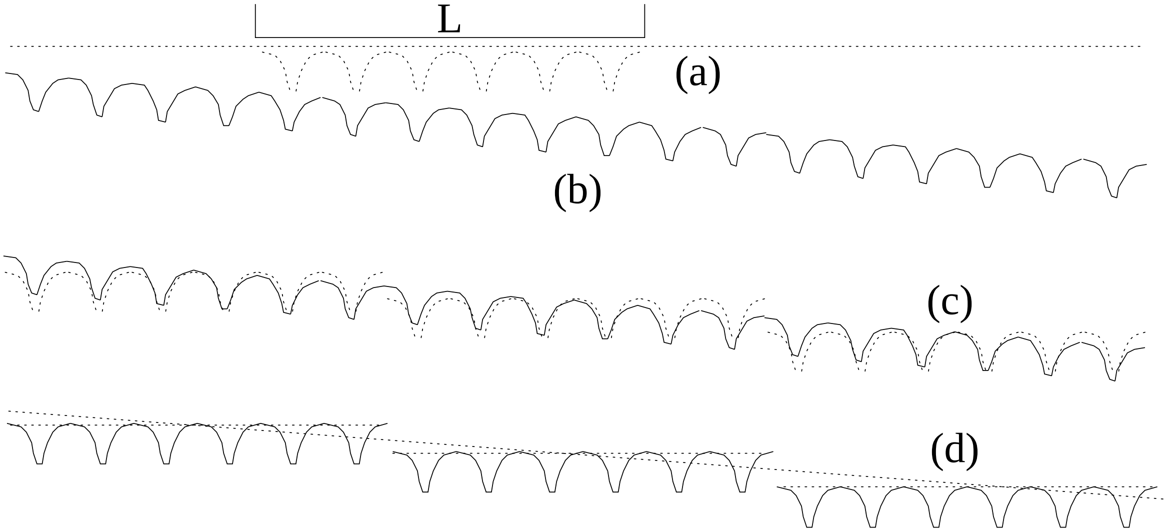

Figure 3: This figure shows a construction of position dependent bands in the presence of an additional potential. The cut (a) shows a region of length L which is "sufficient" to establish a quasicontinuous band. Cut (b) shows the total potential over the region of $n \times L, (n = 3)$. Cut (c) shows that how we can chose a sequence of segments of length L, where each of the centers of the segments we can identify a "local" band structure. Cut (d) shows the stepwise approximation to the total potential. The dotted horizontal lines show a corresponding "approximation" to the macroscopic potential, i.e. as piecewise constant over each segment of length L.

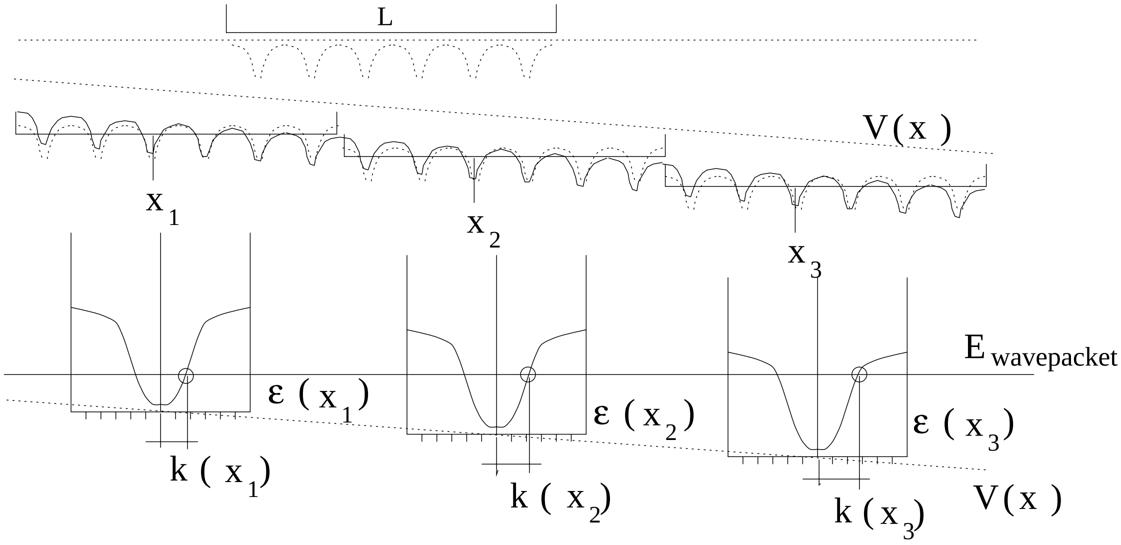

Figure 4: This figure also shows a construction of position dependent bands, but now extended by showing how the other quantities are changing. In particular, it shows why the wavenumber k is function of position, by showing the bands displaced according to the changing potential energy.

i.e.

$$\frac{dk}{dt} = \frac{F}{\hbar}$$

### Effective mass

We continue by considering the time developement of the group velocity. As far as the wavepacket is changing the middle energy $\epsilon(x)$ and wavenumber $\vec{k}(x)$, also the group velocity $\vec{v}_g$ will be changing along $\vec{x}$.
In the following we mean $\vec{v}_g$ when using $\vec{v}$.
In the same way as befoer, we can talk about a time derivative of a quantity, in the sense that the time specifies the position of the wave packet $\vec{x}(t)$.
We thus write

$$\frac{dv_i}{dt} = \frac{d}{dt}\frac{1}{\hbar}\frac{d\epsilon}{dk_i} = \frac{1}{\hbar}\frac{d}{dk_i}\left(\frac{d\epsilon}{dt}\right)$$

To evaluate the Time derivative of $\epsilon$ is the same type of operation as to evaluate the time derivative of the group velocity, our starting point here.
To perform this operation, we consider the variation of $\vec{k}$ with time, i.e.

$$\left(\frac{d\epsilon}{dt}\right) = \left(\sum_{j=1}^{3}\frac{\partial\epsilon}{\partial k_j}\frac{dk_j}{dt}\right)$$

Inserting this paranthesis in the previous equation, we obtain

$$\frac{dv_i}{dt} = \frac{1}{\hbar}\frac{\partial}{\partial k_j}\left(\sum_{j=1}^{3}\frac{\partial\epsilon}{\partial k_j}\frac{dk_j}{dt}\right)$$

Replacing the $dk_j/dt$ by $F_j/\hbar$, we obtain

$$\frac{dv_i}{dt} = \frac{1}{\hbar^2}\sum_{j=1}^{3}\frac{\partial^2\epsilon}{\partial k_i\partial k_j}F_j$$

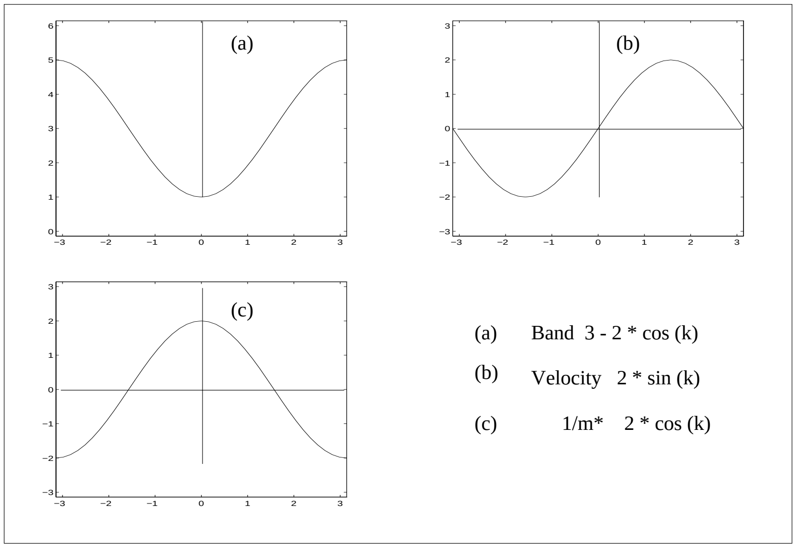

Figure 5: An analytic model for a band - and the concepts of group velocity and effective mass. The meaning of infinite and negative effective mass can be understood from here, consulting also the previous figure. Note that not the effective mass itself, but its inverse $1/m^*$ , is shown.

Inverted mass tensor

$$\mathbf{a} = \left(\frac{1}{\mathbf{m}^*}\right)\mathbf{F}$$

Inverted mass components

$$a_i = \sum_{\mathrm{j}} \left(\frac{1}{m^*}\right)_{\mathrm{i,j}} F_{\mathrm{j}}$$

As partial derivative

$$\left(\frac{1}{m^*}\right)_{i,j} = \frac{1}{\hbar^2}\frac{\partial^2 \varepsilon(\mathbf{k})}{\partial k_i \partial k_j}$$

## Illustrations for the Effective Mass

In the discussion of 3-dimensional bands a very simple expression has been shown to model the structure of the bands, using the trigonometric functions. The following figure illustrates how we can understand the behaviour of the effective mass at the various positions in the band.

The effective mass can be used to describe the density of states in the band. One can use a formula analogous to that one used for the Fermi gas

$$g(\epsilon) = \frac{V}{2\pi^2}\left(\frac{2m^*}{\hbar^2}\right)^{\frac{3}{2}} |\epsilon - \epsilon_b|^{\frac{1}{2}}$$

where $\epsilon_b$ is the minimal or maximal enrgy in the band. Give a short qualitative description of how does the local density of states depend on the shape of the band (as a function of the wavenumber) and how this can be related to the effective mass. Compare qualitatively a narrow and a broad band, considering the density of states as seen from the shape of the $k - \epsilon$ diagram and as seen from the above formula.
The numerical values of the effective mass can even become negative or infinite. Explain the physical meaning of these cases, possibly with the help of the figure 5.