Electron movement in a crystal lattice
Energy bands and effective mass

Dr. Miklós Berta

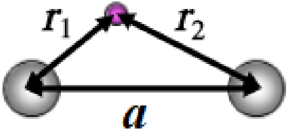
bertam@sze.hu

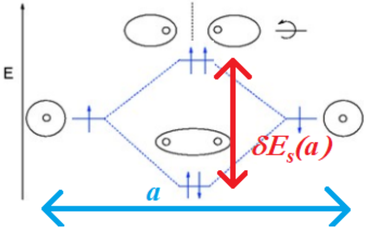
2024. március 18.

SZÉCHENYI ISTVÁN EGYETEM
SZE - GYŐR

Fizika és Kémia Tanszék

H_2^+ - ion





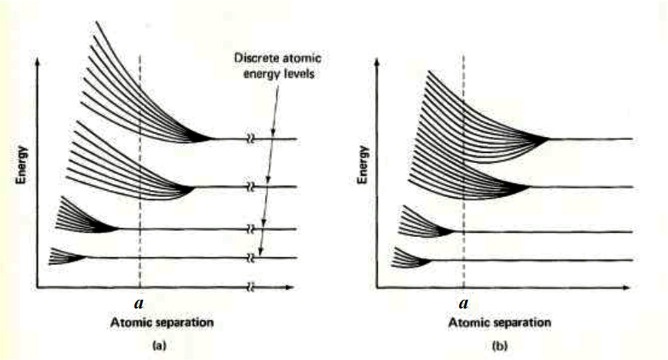
$$\left\{-\frac{\hbar^2}{2m_e}\Delta+\frac{e^2}{4\pi\varepsilon_0}\left(\frac{1}{a}-\frac{1}{r_1}-\frac{1}{r_2}\right)\right\}\psi(\underline{r})=E\psi(\underline{r})$$

$$E_n=E_n^{(0)}\pm\delta E_s(a)$$

$$\psi(\underline{r})\approx c_1\psi_k(\underline{r})+c_2\psi_l(\underline{r})$$

Many electrons in a crystal lattice - Energy bands

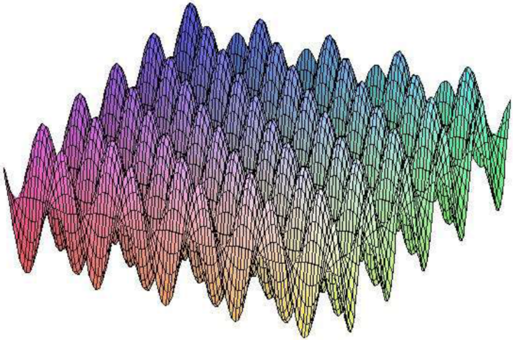
If the lattice constant of the crystal is a, then $2a, 3a, \ldots\ldots, ma$ are also periods. Single-particle energy levels split. The number of split levels is proportional to the number of electrons in the crystal lattice, while the maximum energy splitting is proportional to the lattice constant a.



Based on the Bloch theorem, the state function of the electron in a periodic crystal lattice will also be periodic!

$$\psi(\underline{r}) = \exp\left(i\underline{k}.\underline{r}\right)u(\underline{r}), \;\; \textit{where}$$

$$u(\underline{r}+\underline{a}) = u(\underline{r}) \;\; - \;\; \textit{is } \underline{a} \textit{ periodic.}$$

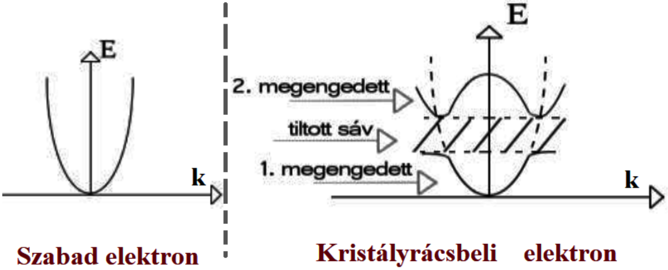


The dispersion – relation specifies how the energy of the electron depends on its momentum.

$$E = f(\underline{p}).$$

For the free electron: $E = \frac{p^2}{2m_e} = \frac{\hbar^2}{2m_e}k^2$

For the electron in a crystal lattice, the dispersion depends on the periodic lattice potential in a more complicated way! $\longrightarrow$ BAND GAP or ENERGY GAP



Effective mass

If a crystal lattice is placed in an external electric field, this field affects the electrons, but the periodic lattice potential also affects them:

$$\boldsymbol{m_e \underline{a}} = \boldsymbol{\underline{F}_{ext}} + \boldsymbol{\underline{F}_{int}}.$$

$$\boldsymbol{m^* \underline{a}} = \boldsymbol{m_e \underline{a}} - \boldsymbol{\underline{F}_{int}} = \boldsymbol{\underline{F}_{ext}}.$$

So, from the point of view of the external field, the electron in the crystal lattice moves like a particle with an effective mass $\boldsymbol{m^*}$.
Electron's effective mass depends on what effect the lattice potential of the crystal lattice has on it!

Thank you!