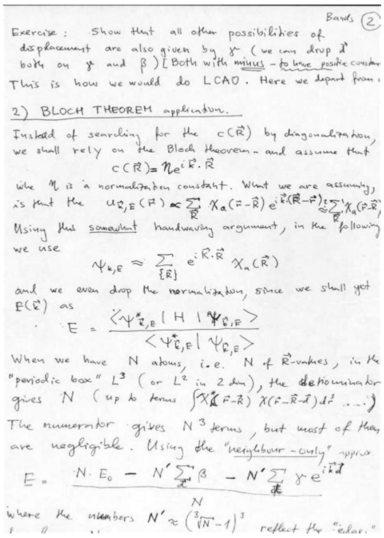

Bands (2)

Exercise: Show that all other possibilities of displacement are also given by γ (we can drop $\vec{d}$ both on γ and β) [Both with minus - to have positive constants]
This is how we would do LCAO. Here we depart from ...

2) BLOCH THEOREM application.

Instead of searching for the $c(\vec{R})$ by diagonalization, we shall rely on the Bloch theorem - and assume that

$$c(\vec{R}) = \eta e^{i\vec{k}\cdot\vec{R}}$$

where η is a normalization constant. What we are assuming, is that the $u_{\vec{k},E}(\vec{r}) \propto \sum_{\vec{R}} \chi_a(\vec{r}-\vec{R}) e^{i\vec{k}\cdot(\vec{R}-\vec{r})} \approx \sum'_{\vec{R}} \chi_a(\vec{r}-\vec{R})$

Using this somewhat handwaving argument, in the following we use

$$\psi_{k,E} \approx \sum_{\{\vec{R}\}} e^{i\vec{k}\cdot\vec{R}} \chi_a(\vec{R})$$

and we even drop the normalization, since we shall get $E(\vec{k})$ as

$$E = \frac{\langle \psi^*_{\vec{k},E} | H | \psi_{\vec{k},E} \rangle}{\langle \psi^*_{\vec{k},E} | \psi_{\vec{k},E} \rangle}$$

When we have N atoms, i.e. N of $\vec{R}$-values, in the "periodic box" L^3 (or L^2 in 2 dim), the denominator gives N (up to terms $\int \chi^*_a(\vec{r}-\vec{R}) \chi(\vec{r}-\vec{R}-\vec{d}) d\vec{r}^3 \ldots$)
The numerator gives N^3 terms, but most of them are negligible. Using the "neighbour-only" approx

$$E = \frac{N \cdot E_0 - N' \sum_{\vec{d}}' \beta - N' \sum_{\vec{d}}' \gamma e^{i\vec{k}\vec{d}}}{N}$$

where the numbers $N' \approx (\sqrt[3]{N} - 1)^3$ reflect the "edges"

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