University of Regensburg | Summer Term 2014

Quantum Theory of Condensed Matter I

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Sheet 2

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1. Tight-binding Hamiltonian in the LCAO basis

In the LCAO method the starting point are the atomic wave functions $\varphi_\nu(\vec{r}-\vec{R}) = \langle \vec{r}|\nu\vec{R}\rangle$, which are solutions of the atomic Schrödinger equation

$$\hat{h}_{\mathrm{at}}|\nu\vec{R}\rangle = \epsilon_\nu|\nu\vec{R}\rangle,$$

with $\hat{h}_{\mathrm{at}} = \hat{p}^2/2m + v_{\mathrm{at}}(\vec{r}-\vec{R})$. This equation describes the interaction of the electron with the potential of an isolated ion at position $\vec{R}$. The Hamiltonian of a particle in a periodic potential can be written as

$$\hat{h} = \frac{\hat{p}^2}{2m} + v(\vec{r}) = \frac{\hat{p}^2}{2m} + \sum_{\vec{R}'} v_{\mathrm{at}}(\vec{r}-\vec{R}') = \hat{h}_{\mathrm{at}} + \Delta v_{\mathrm{at}}(\vec{r}).$$

In the LCAO basis $\hat{h}$ has the general form

$$\hat{h} = \sum_{\nu\nu',\vec{R}\vec{R}'} C_{\nu\vec{R}\nu'\vec{R}'}|\nu\vec{R}\rangle\langle\nu'\vec{R}'|,$$

where $C_{\nu\vec{R}\nu'\vec{R}'} = \langle\nu\vec{R}|\hat{h}|\nu'\vec{R}'\rangle$ are simply the matrix elements of the Hamiltonian in this basis.

1. Express the coefficients $C_{\nu\vec{R}\nu'\vec{R}'}$ in terms of ϵ_ν and $\Delta v_{\mathrm{at}}(\vec{r})$. **(1 Point)**

The tight-binding approximation consists of three assumptions.
(i) The localized atomic orbitals are assumed to satisfy the orthogonality relation $\langle\nu\vec{R}|\nu'\vec{R}'\rangle = \delta_{\nu\nu'}\delta_{\vec{R}\vec{R}'}$.
(ii) Three center integrals are neglected.
(iii) Only nearest neighbours, or up to the next nearest neighbours are retained.

2. Perform the TB approximation and rewrite the $C_{\nu\vec{R}\nu'\vec{R}'}$ using the assumptions (i)-(iii). Keep only the interactions between the nearest neighbours.

   Consider now the LCAO secular equation discussed in the lecture:

   $$\|\epsilon_\nu S_{\nu'\nu} + K_{\nu'\nu} - \epsilon_n(\vec{k})S_{\nu'\nu}\| = 0$$

   What is the form acquired by the overlap integrals $S_{\nu'\nu}$ and $K_{\nu'\nu}$ in the TB approximation? Express them in terms of the coefficients $C_{\nu\vec{R}\nu'\vec{R}'}$ defining the LCAO hamiltonian. **(3 Points)**

3. What is the expression of the secular equation in the TB approximation if only one orbital ν is considered? Calculate the dispersion relation for a homoatomic linear chain with only one orbital per atom and a distance a between the atoms. **(2 Points)**

Frohes Schaffen!