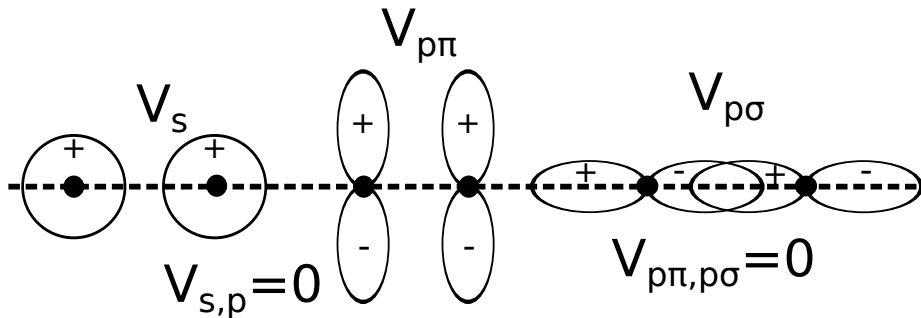


Solid State Theory, Exercises III

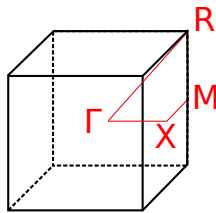
Prof. Hans Peter Büchler SS 2012, 2nd of May 2012

Exercise 1 - Tight Binding Bands in a Cubic Crystal

We will consider the single-electron bands formed in a monoatomic simple cubic crystal, with lattice constant a , from the linear combination of one s and three p orbitals on each atom. The self energies for the s and p orbitals are $\epsilon_s = \langle s_j | \hat{H} | s_j \rangle$ and $\epsilon_p = \langle p_j | \hat{H} | p_j \rangle$. The overlap matrix-elements are $V_s = \langle s_j | \hat{H} | s_{j+1} \rangle$ for two neighboring s orbitals and $V_{p\sigma}$ or $V_{p\pi}$ for two neighboring p orbitals of the same orientation. Note that because of symmetry there is no overlap between s and p or between two neighboring p orbitals of different orientations :



1. What are the signs and relative magnitudes of V_s , $V_{p\sigma}$ and $V_{p\pi}$ when the potential is negative.
2. Using the tight-binding scheme, calculate the four different energy bands and their bandwidths along the directions $\vec{k} = (k, 0, 0)$, $\vec{k} = (k, k, 0)$ and $\vec{k} = (k, k, k)$. You should assume that the self energies of the s and p orbitals are different enough, $\epsilon_p > \epsilon_s$, that we can ignore $s - p$ mixing.
3. Sketch the band structure along the lines : $\Gamma - X - M - R - \Gamma$ (these points on the reciprocal lattice are shown below). Comment on how strongly the s and p orbitals are likely to mix.



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Exercise 2 - Electronic Density of States

Consider the following tight binding dispersion

$$E(\mathbf{k}) = -2t \sum_{i=1}^d \cos(k_i a), \quad (1)$$

where t is the hopping integral and a is the lattice spacing.

1. Calculate the density of states for $d = 1$ and discuss the algebraic form of the van Hove singularities at $E = \pm 2t$.
2. Make a drawing of the DOS in $d = 3$. Using the tight binding dispersion in Eq. (1), calculate the number of possible van Hove points in $d = 3$, and then use a parabolic approximation for the dispersion around such points and calculate the DOS.

*Observe that the DOS is free of van Hove singularities in the limit $d \rightarrow \infty$. In fact, if we consider the sum over \mathbf{k} points in the DOS as a sum over randomly chosen numbers $-2t \cos(k_i a)$, then the **central limit theorem** tells us that in the limit $d \rightarrow \infty$ the DOS becomes a Gaussian, thus free of singularities.*

Solutions due on : 9th of May, 2012