https://www2.physik.uni-muenchen.de/lehre/vorlesungen/wise_24_25/TA1_theoretical_condensed_matter/index.html

Problem set 8

Problem 1 Crystal-field splitting

In the lecture we discussed the tight-binding approximation for the case of only one atomic orbital. Now, we want to extend the problem to multi-band models, which, for instance, are important for the transition-metal oxides. Consider the eigenfunctions $\langle r, \vartheta, \varphi | \psi_{nlm} \rangle = R_{nl}(r) Y_l^m(\vartheta, \varphi)$ of a Hamiltonian with rotational invariant potential $V(|\hat{\vec{r}}|)$ (e.g., the Hydrogen problem), where $R_{nl}(r)$ denotes the radial wavefunction and $Y_l^m(\vartheta, \varphi)$ the spherical harmonics, describing the angular dependency. In a typical transition-metal oxide, each transition-metal atom is surrounded by oxygen atoms which, due to orbital hybridization, exhibit only an imperfectly screening of the charged nuclei. In such a situation, the potential $V(|\hat{\vec{r}}|)$ is perturbed by the effective excess charges of the oxygen nuclei and we assume a perturbation of the form

$$\Delta V(\hat{\vec{r}}) = \lambda \left(\hat{x}^4 + \hat{y}^4 + \hat{z}^4 \right) , \tag{1}$$

where $\lambda > 0$.

(1.a) Show that the perturbation $\Delta V(\hat{\vec{r}})$ breaks the full rotational symmetry of the original problem down to a cubic symmetry.

(1.b) For the d-orbitals ($l = 2$), compute the energy corrections arising from $\Delta V(\hat{\vec{r}})$ to first order in degenerate perturbation theory. Show that the five-fold degeneracy of the d-orbitals is split into two levels with a three- and a two-fold degeneracy.

Problem 2 Beyond Graphene

In the lecture, we discussed graphene's band structure using the tight-binding model on a honeycomb lattice, with nearest-neighbor hopping t. Now, we want to consider the same model, but add a site-dependent energy for the local orbital, that has the value $+V$ for all A sublattice sites and $-V$ for all B sublattice sites.

(2.a) Calculate the band dispersions in this case, and in particular the band gap.

(2.b) Show that, when $V \neq 0$, a mass term is added to the Dirac Hamiltonian $\hat{H} = v_{\mathrm{F}}(\tau_z \sigma_x \hat{p}_x + \sigma_y \hat{p}_y)$, and calculate this mass as well as its relation to the band gap.