Exercises for Theoretical Condensed Matter (WS 1718)
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Exercise-sheet 4 (November 10, 2017)

1 In-class exercises

1.1 DOS of the tight-binding model on the infinite-dimensional hypercube

The tight-binding model on a d-dimensional hypercube has the dispersion

$$\epsilon(\boldsymbol{k}) = -2t \sum_{j=1}^{d} \cos k_j a, \tag{1}$$

where a is the lattice constant and t is the hopping amplitude. It follows from equation (1) that the band edges lie at $\pm 2td$.

(a) How should the hopping parameter t scale with d so that the kinetic energy remains finite in the limit $d \to \infty$?

(b) Show that there are no van Hove singularities for the tight-binding model on the infinite-dimensional hypercube.

2 Homework - due date: November 17, 2017 (35 + 5 points).

2.1 The CuO_2 lattice (15 points)

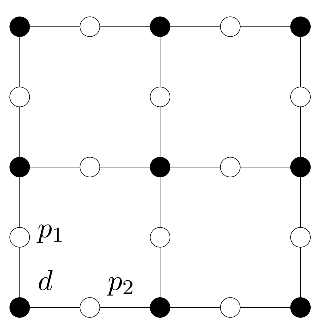

Figure 1: CuO_2 lattice.

Let us consider a simplified picture of the CuO_2 planes in La_2CuO_4, where we replace the actual oxygen p- and Cu d-orbitals with s-orbitals, and neglect the direct hopping between oxygen atoms. The unit-cell of the lattice contains three atoms (see Fig. 1), and the nearest-neighbour distance between each O and Cu atom is a.

Let the corresponding Wannier states be created by the fermionic operators $d^\dagger_{\boldsymbol{j},\sigma}$, $p^\dagger_{1\boldsymbol{j},\sigma}$ and $p^\dagger_{2\boldsymbol{j},\sigma}$, respectively, where σ labels the spin. The tight-binding Hamiltonian can then be written as

$$\begin{aligned} H \;=\; & \sum_{\boldsymbol{j},\sigma} \Big[\epsilon_d \, d^\dagger_{\boldsymbol{j},\sigma} d_{\boldsymbol{j},\sigma} + \epsilon_p \left(p^\dagger_{1\boldsymbol{j},\sigma} p_{1\boldsymbol{j},\sigma} + p^\dagger_{2\boldsymbol{j},\sigma} p_{2\boldsymbol{j},\sigma} \right) \\ & -t \left(d^\dagger_{\boldsymbol{j},\sigma} p_{1\boldsymbol{j},\sigma} + d^\dagger_{\boldsymbol{j},\sigma} p_{2\boldsymbol{j},\sigma} + d^\dagger_{\boldsymbol{j}+\boldsymbol{y},\sigma} p_{1\boldsymbol{j},\sigma} + d^\dagger_{\boldsymbol{j}+\boldsymbol{x},\sigma} p_{2\boldsymbol{j},\sigma} \right) + h.c. \Big] , \end{aligned} \tag{2}$$

where $\boldsymbol{x}$ and $\boldsymbol{y}$ are the elementary lattice translation vectors.

(a) Show that the spectrum of the model consists of three bands, one of which is flat whereas the other two have the form

$$\lambda^\pm(\boldsymbol{k}) = \frac{\epsilon_p + \epsilon_d}{2} \pm \sqrt{\frac{(\epsilon_p - \epsilon_d)^2}{4} + \Delta(\boldsymbol{k})}, \tag{3}$$

with $\Delta(\boldsymbol{k})$ a hybridization function to be determined.

(b) (BONUS + 5 points) At half-filling, what can you say about the spin degeneracy of the ground state if $\epsilon_d = \epsilon_p = 0$?

2.2 van Hove singularity of the tight-binding model on the square lattice (10 points)

The density of states was defined in the lecture to be

$$\rho_n(\epsilon) = \frac{2}{N} \sum_{\boldsymbol{k}} \delta(\epsilon - \epsilon_n(\boldsymbol{k})), \tag{4}$$

where $\boldsymbol{k}$ lies on the first Brillouin zone and $\epsilon_n(\boldsymbol{k})$ is the dispersion relation of the nth band.

(a) Show that one can also represent the density of states as the surface integral

$$\rho_n(\epsilon) = \int_{S_n(\epsilon)} \frac{2}{(2\pi)^d} \frac{dS}{|\boldsymbol{\nabla} \epsilon_n(\boldsymbol{k})|}. \tag{5}$$

(b) Use equation (5) together with an approximate form of the "equipotential" ϵ lines in $\boldsymbol{k}$-space to derive the van Hove singularities for the tight-binding band of a square lattice.

2.3 Density of states of a photon mode of a 2D system (10 points)

Let us consider a square lattice with a single phonon mode of dispersion relation

$$\omega^2 = \omega_0^2 \left(2 - \cos k_x - \cos k_y\right) \tag{6}$$

(a) Compute the density of states numerically by using equation (4).

(b) Consider the small-wavelength expansion $\omega = \omega_0 |\boldsymbol{k}|/\sqrt{2}$. Find the corresponding DOS (analytically) and plot it together with the result obtained in (a).