

Exercise-sheet 4 (November 16, 2015)

1 In-class exercises

1.1 van Hove singularity of the tight-binding model on the square lattice

The density of states was defined in the lecture to be

$$\rho_n(\epsilon) = \frac{2}{N} \sum_{\mathbf{k}} \delta(\epsilon - \epsilon_n(\mathbf{k})), \quad (1)$$

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

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

$$\rho_n(\epsilon) = \int_{S_n(\epsilon)} \frac{2}{(2\pi)^d} \frac{dS}{|\nabla \epsilon_n(\mathbf{k})|} \quad (2)$$

- (b) Use equation (2) to derive the van Hove singularities for the tight-binding band of a square lattice.

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

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

$$\epsilon(\mathbf{k}) = -2t \sum_{j=1}^d \cos k_j a, \quad (3)$$

where a is the lattice constant and t is the hopping amplitude. It follows from equation (3) 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 $d \rightarrow \infty$?
- (b) Show that there are no van Hove singularities for the tight-binding model on the infinite-dimensional hypercube.

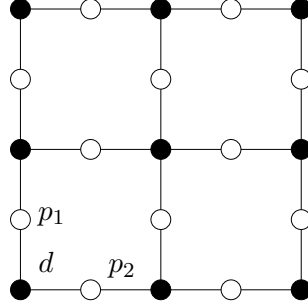


Figure 1: CuO₂ lattice.

2 Homework - due date: November 23, 2015 (30 points).

2.1 The CuO₂ lattice (15 points)

Let us consider a simplified picture of the CuO₂ planes in La₂CuO₄, 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 $d_{j,\sigma}^\dagger$, $p_{1j,\sigma}^\dagger$ and $p_{2j,\sigma}^\dagger$, respectively, where σ labels the spin. The tight-binding Hamiltonian can then be written as

$$H = \sum_{j,\sigma} \left[\epsilon_d d_{j,\sigma}^\dagger d_{j,\sigma} + \epsilon_p \left(p_{1j,\sigma}^\dagger p_{1j,\sigma} + p_{2j,\sigma}^\dagger p_{2j,\sigma} \right) - t \left(d_{j,\sigma}^\dagger p_{1j,\sigma} + d_{j,\sigma}^\dagger p_{2j,\sigma} + d_{j+\mathbf{y},\sigma}^\dagger p_{1j,\sigma} + d_{j+\mathbf{x},\sigma}^\dagger p_{2j,\sigma} \right) + h.c. \right], \quad (4)$$

where \mathbf{x} and \mathbf{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

$$\lambda^\pm(\mathbf{k}) = \frac{\epsilon_p + \epsilon_d}{2} \pm \sqrt{\frac{(\epsilon_p - \epsilon_d)^2}{4} + \Delta(\mathbf{k})}, \quad (5)$$

with $\Delta(\mathbf{k})$ 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 Density of states for hybridized bands (5 points)

Consider the situation in which electrons can jump from a broad band $\epsilon(\mathbf{k})$ and a narrow energy level ϵ_0 . The hybridized energy levels can be computed as

$$\tilde{\epsilon} = \frac{\epsilon + \epsilon_0}{2} \pm \sqrt{\frac{(\epsilon - \epsilon_0)^2}{4} + \Delta}, \quad (6)$$

with Δ a hybridization constant. Assume the ϵ band has a constant DOS $\rho(\epsilon) = \rho_0$ over a bandwidth $W = \epsilon_2 - \epsilon_1$, so that $\rho(\epsilon) = 0$ for $\epsilon < \epsilon_1$ or $\epsilon > \epsilon_2$. Likewise assume that for the narrow band, the DOS peaks sharply at ϵ_0 , i.e. $\rho(\epsilon) = \rho_0 W \delta(\epsilon - \epsilon_0)$.

Calculate the DOS for the hybridized band, its bandwidth and where it vanishes using

$$\rho(\tilde{\epsilon}) = \rho(\epsilon) \frac{d\epsilon}{d\tilde{\epsilon}}. \quad (7)$$

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

$$\omega^2 = \omega_0^2 (2 - \cos k_x - \cos k_y) \quad (8)$$

- (a) Compute the density of states numerically by using equation (1).
- (b) Consider the small-wavelength expansion $\omega = \omega_0 |\mathbf{k}| / \sqrt{2}$. Find the corresponding DOS (analytically) and plot it together with the result obtained in (a).