

Problem 1. Lattice Dirac model

Implement the Lattice Dirac model. This is the fixed spin sector or the Bernevig-Hughes-Zhang model discussed in the lecture:

$$H = \begin{pmatrix} m + \cos k_x + \cos k_y & \sin k_x - i \sin k_y \\ \sin k_x + i \sin k_y & -m - \cos k_x - \cos k_y \end{pmatrix} \quad (1)$$

1. Study the spectrum of the system as a function of m . For which coupling do you observe a closure of the gap?
2. For different values of m , study the character of the bands along a high symmetry line of the Brillouin zone. Do you observe band inversion?
3. Consider an cylinder geometry, where k_y is still a good quantum number. Compare the spectrum of an open and periodic geometry along x for different values of m and sample length $L_x = 50$.

You should be able to reproduce the results and figures presented in the lecture notes.

Problem 2. Hohenberg-Kohn theorems

Give a proof of the two Hohenberg-Kohn theorems seen in the lecture.

1. The total energy of an electronic system in an external potential $V_{ne}(\mathbf{r})$ is a unique functional of the electron density $\rho(\mathbf{r})$:

$$E[\rho] = \int d^3\mathbf{r} V_{ne}(\mathbf{r})\rho(\mathbf{r}) + F[\rho], \quad (2)$$

where $F[\rho]$ is an unknown, but otherwise universal functional of the electron density $\rho(\mathbf{r})$ only.

Hint: Proceed by *reductio ad absurdum*.

2. The density that minimises the total energy is the groundstate density $\rho_0(\mathbf{r})$. The corresponding energy is the groundstate energy E_0 .

$$E[\rho] \geq E[\rho_0] = E_0. \quad (3)$$

Hint: Start from the variational principle for wavefunctions: $E_0 \leq \langle \psi | H | \psi \rangle$.