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Topological condensed matter physics
Problem set 1

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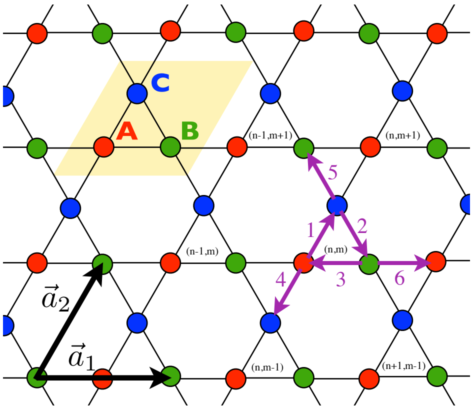
1. Tight-binding band structure of the Kagome lattice — 2 Points

Investigate the so-called Kagome lattice, a hexagonal, two-dimensional lattice with a three-atomic basis ("Kagome" originally denotes Japanese bamboo baskets with precisely this pattern).



To calculate the tight-binding band structure of the Kagome lattice, analyze a hopping between nearest neighbor sites. The associated Hamiltonian is thus of the form $H_K = \sum_{<ij>} c_i^\dagger c_j + \text{H.c.}$, where $< ij >$ denotes nearest neighbor sites i and j, while c_i is the electronic annihilation operator on site i. The primitive unit vectors are $\boldsymbol{a}_1 = a(1,0)$ and $\boldsymbol{a}_2 = a(1/2, \sqrt{3}/2)$, and a is the microscopic lengthscale of the lattice. The basis is given by the vectors $\boldsymbol{r}_1 = 0$ (A, red), $\boldsymbol{r}_2 = \boldsymbol{a}_1/2$ (B, green), and $\boldsymbol{r}_3 = \boldsymbol{a}_2/2$ (C, blue). Every small triangle with a tip to the top is thus a unit cell, which can be indexed by (n, m) as indicated in the figure. To simplify the notation, use operators A_{nm}, B_{nm}, and C_{nm} to annihilate electrons in the respective sites of unit cell (n, m) (instead of c_i). The Hamiltonian thus takes the form

$$H_K = t \sum_{n,m} \left[C_{nm}^\dagger A_{nm} + B_{nm}^\dagger C_{nm} + A_{nm}^\dagger B_{nm} + C_{n(m-1)}^\dagger A_{nm} + B_{(n-1)(m+1)}^\dagger C_{nm} + A_{(n+1)m}^\dagger B_{nm} + \text{H.c.} \right] \tag{1}$$

Rewrite the Hamiltonian as a (3×3)-matrix, and find its eigenvalues by Fourier transformation. Plot and discuss the resulting energy spectrum.

Hint: you may use

$$\cos^2\left(\frac{\boldsymbol{k}\cdot\boldsymbol{a}_1}{2}\right) + \cos^2\left(\frac{\boldsymbol{k}\cdot\boldsymbol{a}_2}{2}\right) + \cos^2\left(\frac{\boldsymbol{k}\cdot(\boldsymbol{a}_1-\boldsymbol{a}_2)}{2}\right) = 2\cos\left(\frac{\boldsymbol{k}\cdot\boldsymbol{a}_1}{2}\right)\cos\left(\frac{\boldsymbol{k}\cdot\boldsymbol{a}_2}{2}\right)\cos\left(\frac{\boldsymbol{k}\cdot(\boldsymbol{a}_1-\boldsymbol{a}_2)}{2}\right) + 1$$

2. Berry curvature of a two-band Hamiltonian **4 Points**

Consider a Hamiltonian $H(\mathbf{R})$ with eigenstates $|n(\boldsymbol{R})\rangle$ of energy $E_n(\boldsymbol{R})$, which depends on a real three-dimensional vector of parameters $\boldsymbol{R}$. The Berry curvature pseudovector (effective magnetic field) $\mathbf{V}_n$ associated with $|n(\boldsymbol{R})\rangle$ is given by

$$\mathbf{V}_n = -\mathrm{Im}\,\langle \nabla_{\boldsymbol{R}} n(\boldsymbol{R})| \times |\nabla_{\boldsymbol{R}} n(\boldsymbol{R})\rangle = \hat{e}_i\,\mathrm{Im}\,\epsilon_{ijk} \sum_{m\neq n} \frac{\langle n(\boldsymbol{R})|\,(\nabla_{R_j} H)\,|m(\boldsymbol{R})\rangle\,\langle m(\boldsymbol{R})|\,(\nabla_{R_k} H)\,|n(\boldsymbol{R})\rangle}{(E_m(\boldsymbol{R}) - E_n(\boldsymbol{R}))^2} \tag{2}$$

In the following, we will more specifically analyze the general two-band Hamiltonian

$$H(\boldsymbol{R}) = a(\boldsymbol{R})\mathbb{1}_{2\times 2} + \boldsymbol{d}(\boldsymbol{R}) \cdot \boldsymbol{\sigma}\ , \tag{3}$$

where $\boldsymbol{\sigma}$ is the vector of Pauli matrices, and where the scalar $a(\boldsymbol{R})$ and vector $\boldsymbol{d}(\boldsymbol{R})$ are both real functions of $\boldsymbol{R}$.

a) **1 Point**

Why can you calculate the Berry curvature associated with eigenstates of $H(\boldsymbol{R})$ (with $\boldsymbol{d}(\boldsymbol{R}) \neq 0$) also from the Hamiltonian

$$\tilde{H}(\boldsymbol{R}) = \hat{\boldsymbol{d}}(\boldsymbol{R}) \cdot \boldsymbol{\sigma} \tag{4}$$

with $\hat{\boldsymbol{d}}(\boldsymbol{R}) = \boldsymbol{d}(\boldsymbol{R})/|\boldsymbol{d}(\boldsymbol{R})|$?

b) **1 Point**

Show that the i^{th} component of the Berry curvature pseudovector associated with $|n(\boldsymbol{R})\rangle$ can also be calculated as

$$\mathbf{V}_{n,i} = \frac{1}{4}\mathrm{Im}\ \epsilon_{ijk}\,\langle n(\boldsymbol{R})|\,(\nabla_{R_j}\tilde{H})\,(\nabla_{R_k}\tilde{H})\,|n(\boldsymbol{R})\rangle\,. \tag{5}$$

c) **1 Point**

Use $\sigma_\alpha\sigma_\beta = \mathbb{1}_{2\times 2}\delta_{\alpha\beta} + i\epsilon_{\alpha\beta\gamma}\sigma_\gamma$ to show that the Berry curvature associated with $|-(\boldsymbol{R})\rangle$, the eigenstate of the the lower band, can be obtained from

$$\mathbf{V}_{-,i} = \frac{1}{4}\epsilon_{ijk}\ \epsilon_{\alpha\beta\gamma}\ (\nabla_{R_j}\hat{d}_\alpha(\boldsymbol{R}))\,(\nabla_{R_k}\hat{d}_\beta(\boldsymbol{R}))\,\mathrm{Re}\,\langle -(\boldsymbol{R})|\,\sigma_\gamma\,|-(\boldsymbol{R})\rangle\,. \tag{6}$$

d) **1 Point**

Parametrizing $\hat{\boldsymbol{d}}(\boldsymbol{R}) = \begin{pmatrix} \sin(\theta)\cos(\phi) \\ \sin(\theta)\sin(\phi) \\ \cos(\theta) \end{pmatrix}$, where ϕ and θ are functions of $\boldsymbol{R}$, the analogy to eigenstates of the spin operator along some general direction implies $|-(\boldsymbol{R})\rangle = \begin{pmatrix} \sin(\theta/2) \\ -\cos(\theta/2)e^{i\phi} \end{pmatrix}$. You may use the addition theorems $2\sin(x)\cos(x) = \sin(2x)$ and $\cos^2(x) - \sin^2(x) = \cos(2x)$ to show that

$$\mathbf{V}_{-,i} = -\frac{1}{4}\epsilon_{ijk}\ \hat{\boldsymbol{d}}(\boldsymbol{R}) \cdot (\nabla_{R_j}\hat{\boldsymbol{d}}(\boldsymbol{R})) \times (\nabla_{R_k}\hat{\boldsymbol{d}}(\boldsymbol{R})). \tag{7}$$

3. Domain wall bound state in the SSH-model **2 Points**

a) **1 Point**

Starting from the time-independent Schrödinger equation of a general second-quantized fermionic (2×2)-Hamiltonian,

$$H = \int dx (c_1^\dagger(x), c_2^\dagger(x)) \begin{pmatrix} h_{11}(x) & h_{12}(x) \\ h_{21}(x) & h_{22}(x) \end{pmatrix} \begin{pmatrix} c_1(x) \\ c_2(x) \end{pmatrix} \tag{8}$$

where $c_{1,2}(x)$ are annihilation operators, use the ansatz

$$|\Psi\rangle = \int dx \, \Big(u(x) c_1^\dagger(x) + v(x) c_2^\dagger(x) \Big) |0\rangle, \tag{9}$$

where $|0\rangle$ is the vacuum defined by $c_{1,2}(x)|0\rangle = 0$, to obtain a matrix equation for the coefficients $u(x)$ and $v(x)$.

b) **1 Point**

For one spin species, a continuum version of the (infinitely long) SSH model is described by the Hamiltonian

$$H_{\text{SSH}} = \int dx \, \Psi^\dagger(x)(-iv_F \partial_x \sigma_x + m(x)\sigma_y)\Psi(x) \tag{10}$$

(in the lecture, the Fermi velocity v_F and mass m were given by $v_F = -ta$ and $m = 2\delta t$). $\Psi(x)$ is a spinor of two different annihilation operators. Assuming that the mass is a monotonically increasing function with a sign change at $x = 0$,

$$m(x<0) < 0 \quad , \quad m(x=0) = 0 \quad , \quad m(x>0) > 0 \; , \tag{11}$$

find the zero-energy bound state(s) associated with the domain wall. How many are there?