1. Tight-binding band structure of the Kagome lattice

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 \( \mathbf{a}_1 = a(1,0) \) and \( \mathbf{a}_2 = a(1/2, \sqrt{3}/2) \), and \( a \) is the microscopic lengthscale of the lattice. The basis is given by the vectors \( \mathbf{r}_1 = 0 \) (A, red), \( \mathbf{r}_2 = \mathbf{a}_1/2 \) (B, green), and \( \mathbf{r}_3 = \mathbf{a}_2/2 \) (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

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

(1)

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

Hint: you may use

\[ \cos^2 \left( \frac{k \cdot \mathbf{a}_1}{2} \right) + \cos^2 \left( \frac{k \cdot \mathbf{a}_2}{2} \right) + \cos^2 \left( \frac{k \cdot (\mathbf{a}_1 - \mathbf{a}_2)}{2} \right) = 2 \cos \left( \frac{k \cdot \mathbf{a}_1}{2} \right) \cos \left( \frac{k \cdot \mathbf{a}_2}{2} \right) \cos \left( \frac{k \cdot (\mathbf{a}_1 - \mathbf{a}_2)}{2} \right) + 1 \]
2. Berry curvature of a two-band Hamiltonian

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

\[
V_n = -\text{Im} \left( \nabla_R n(R) | \nabla_R n(R) \right) = \epsilon_i \text{Im} \sum_{m \neq n} \frac{\langle n(R) | (\nabla_{R_j} H) | m(R) \rangle \langle m(R) | (\nabla_{R_k} H) | n(R) \rangle}{(E_m(R) - E_n(R))^2}
\]  

(2)

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

\[
H(R) = a(R) 1_{2 \times 2} + d(R) \cdot \sigma ,
\]

(3)

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

a) 1 Point

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

\[
\tilde{H}(R) = \hat{d}(R) \cdot \sigma
\]

(4)

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

b) 1 Point

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

\[
V_{n,i} = \frac{1}{4} \text{Im} \epsilon_{ijk} \langle n(R) | (\nabla_{R_j} \tilde{H}) (\nabla_{R_k} \tilde{H}) | n(R) \rangle .
\]

(5)

c) 1 Point

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

\[
V_{-,i} = \frac{1}{4} \epsilon_{ijk} \epsilon_{\alpha\beta\gamma} \langle \nabla_{R_j} \hat{d}_\alpha(R) \rangle \langle \nabla_{R_k} \hat{d}_\beta(R) \rangle \text{Re} \langle -\langle R\rangle | \sigma_\gamma | -\langle R\rangle \rangle .
\]

(6)

d) 1 Point

Parametrizing \( \hat{d}(R) = \begin{pmatrix} \sin(\theta) \cos(\phi) \\ \sin(\theta) \sin(\phi) \\ \cos(\theta) \end{pmatrix} \), where \( \phi \) and \( \theta \) are functions of \( R \), the analogy to eigenstates of the spin operator along some general direction implies \( |-\langle R\rangle\rangle = \begin{pmatrix} \sin(\theta/2) \\ -\cos(\theta/2)e^{i\phi} \end{pmatrix} \). 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

\[
V_{-,i} = -\frac{1}{4} \epsilon_{ijk} \hat{d}(R) \cdot (\nabla_{R_j} \hat{d}(R)) \times (\nabla_{R_k} \hat{d}(R)) .
\]

(7)
3. Domain wall bound state in the SSH-model  

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

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

(8)

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

\[ |\Psi\rangle = \int dx \left( u(x)c_1^\dagger(x) + v(x)c_2^\dagger(x) \right) |0\rangle, \]  

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

\[ H_{SSH} = \int dx \Psi^\dagger(x)(-iv_F\partial_x\sigma_x + m(x)\sigma_y)\Psi(x) \]  

(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 $x = 0$,

\[ m(x < 0) < 0 \quad m(x = 0) = 0 \quad m(x > 0) > 0, \]  

(11)

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