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Theory of Frustrated Magnetism
Problem set 1

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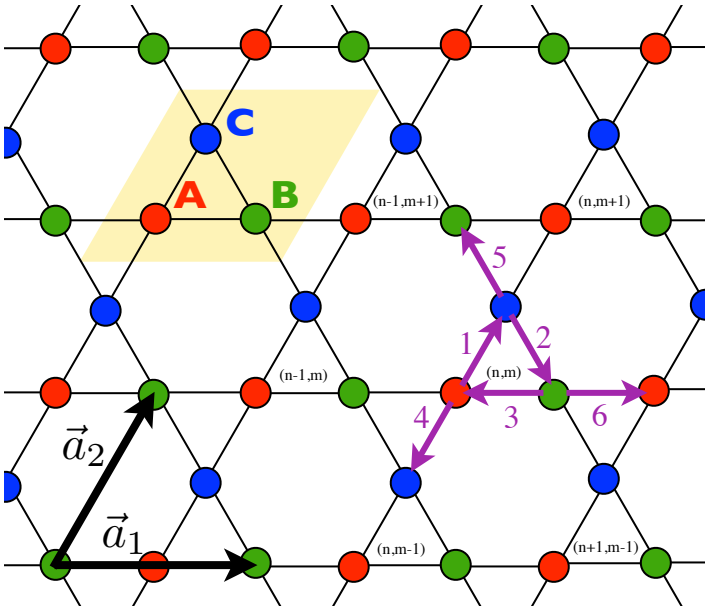
1. Tight-Binding Bands of the Kagome Lattice — 7 Points

Consider the Kagome lattice shown below which forms a two-dimensional hexagonal net with a three-atomic unit cell ("kagome" is the japanese word for a traditional basket with such a pattern).



Compute the bandstructure for a nearest-neighbor tight-binding model for spinless fermions on the Kagome lattice.

Guideline: The Hamiltonian can be written as $H_K = -t\sum_{\langle ij\rangle}(c_i^\dagger c_j + \text{h.c.})$. The primitive lattice vectors are given by $\boldsymbol{a}_1 = a(1,0)$ and $\boldsymbol{a}_2 = a(1/2,\sqrt{3}/2)$. The basis atoms are located at $\boldsymbol{r}_1 = 0$ (A/red), $\boldsymbol{r}_2 = \boldsymbol{a}_1/2$ (B/green) und $\boldsymbol{r}_3 = \boldsymbol{a}_2/2$ (C/blue). The unit cell is indicated by the yellow rhomboid. In the following, each unit cell will be labeled with x and y coordinates (n,m), see above. Instead of $c_j^{(\dagger)}$ we are using the operators $A_{(n,m)}^{(\dagger)}$, $B_{(n,m)}^{(\dagger)}$, $C_{(n,m)}^{(\dagger)}$, which annihilate (create) an electron on the corresponding sublattice A, B, C within the (n,m)-th unit cell. Thus we can write all nearest-neighbor hopping processes (see purple arrows above plus hermitian conjugation) as

$$H_K = -t\sum_{n,m}\Big[C_{n,m}^\dagger A_{n,m} + B_{n,m}^\dagger C_{n,m} + A_{n,m}^\dagger B_{n,m} + C_{n,m-1}^\dagger A_{n,m} + B_{n-1,m+1}^\dagger C_{n,m} + A_{n+1,m}^\dagger B_{n,m} + \text{h.c.}\Big] \tag{1}$$

The Fourier transform of these terms can be conveniently arranged into a 3×3 matrix, the Bloch matrix, and its eigenvalues are the energy bands. Calculate and sketch these bands in the Brillouin zone.

Hint: Determine the characteristic equation of the 3×3 matrix and use the identity

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

One of the eigenvalues has a simple form which you might guess.

2. Strong-Coupling Limit of the Hubbard Model — 11 Points

Consider a real nearest-neighbor hopping on an arbitrary lattice,

$$H_0 = \sum_{\langle ij \rangle} h_{ij} \quad \text{with} \quad h_{ij} = -t \sum_{\sigma=\uparrow,\downarrow} \left(c^\dagger_{i\sigma} c_{j\sigma} + \text{h.c.} \right) \tag{2}$$

If we want to describe the effect of Coulomb repulsion between the electrons, this can be accomplished in the simplest way using the Hubbard interaction,

$$H_I = U \sum_i n_{i\uparrow} n_{i\downarrow} \ , \tag{3}$$

where $n_{i\sigma} = c^\dagger_{i\sigma} c_{i\sigma}$ is the number operator. At half filling, *i.e.*, one particle per lattice site, and for strong U hopping processes of the electrons are suppressed. This is the strong-coupling limit where only the spin degree of freedom of the electrons remains at low energies.

a) **5 Points**

Show that, for very large U at half filling, $H = H_0 + H_I$ corresponds to the low-energy spin Hamiltonian

$$H_{\text{spin}} = J \sum_{\langle ij \rangle} \left[\frac{1}{2} \left(S^+_i S^-_j + S^-_i S^+_j \right) + S^z_i S^z_j - \frac{1}{4} \right] \tag{4}$$

with $J = (4t^2)/U$. This is the isotropic Heisenberg model.

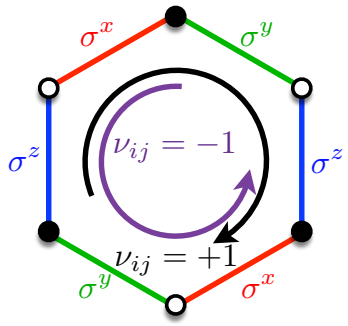
Guideline: Note that formally one has to perform second-order perturbation theory in $1/U$, *i.e.*, $H_{\text{spin}} = -\boldsymbol{T}\boldsymbol{U}^{-1}\boldsymbol{T}^\dagger$ where $\boldsymbol{T}$ and $\boldsymbol{U}$ are matrices. Consider two sites for which the low-energy states $|s\rangle$ at half filling are singly occupied, $|s\rangle \in \{|\uparrow,\uparrow\rangle, |\uparrow,\downarrow\rangle, |\downarrow,\uparrow\rangle, |\downarrow,\downarrow\rangle\}$. Virtual hopping processes result in states $|d\rangle \in \{|\uparrow\downarrow,0\rangle, |0,\uparrow\downarrow\rangle\}$ where one site is empty and the other doubly occupied. Matrix elements of $\boldsymbol{T}$ are given by $\langle s| h_{12} |d\rangle$ and of $\boldsymbol{U}$ by $\langle d| H_I |d\rangle$. In general, we expect in second-order perturbation theory an effective spin Hamiltonian with matrix elements $\langle s| J^{\mu\mu'} S^\mu_1 S^{\mu'}_2 |s'\rangle + c\,\delta_{ss'}$ $(\mu = x, y, z)$ which can be compared with the matrix elements of H_{spin}. The constant c sets the energy zero point. The use of ladder operators $S^\pm_j = S^x_j \pm i S^y_j$ might be helpful.

b) **3 Points**

How does the resulting spin Hamiltonian change when imaginary, spin-dependent hopping is considered instead of (2)? As an concrete example, consider the spin-orbit type term on the honeycomb lattice

$$H'_0 = i\lambda \sum_{\langle ij \rangle_\mu} \nu_{ij} c^\dagger_{i\alpha} \sigma^\mu_{\alpha\beta} c_{j\beta} \ . \tag{5}$$

Nearest-neighbor bonds $\langle ij \rangle_\mu$ differ now by the involved Pauli matrices σ^μ as indicated in the figure below; $\nu_{ij} = \pm 1$ depending on whether hopping is clockwise ($\nu_{ij} = +1$) or counter-clockwise ($\nu_{ij} = -1$).



Perform the calculation for one of the three different bonds (blue, red, or green) and guess the solution of the others.

c) **3 Points**

Now repeat the calculation for a Hubbard model with both kinetic terms, *i.e.*, $\tilde{H} = H_0 + H'_0 + H_I$.