Renormalization Group Analysis of Nb_3Cl_8

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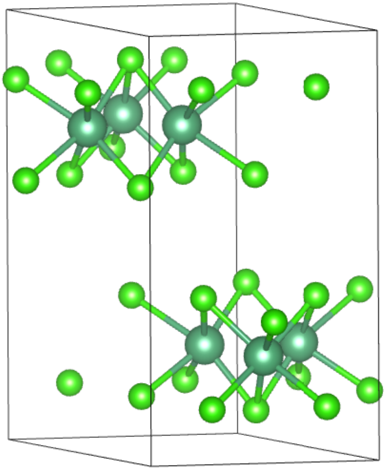
System



- **Component**: 2-class **Nb** d-orbitals
  1. $\{d_{z^2}\}$
  2. $\{d_{x^2-y^2}, d_{xy};\ d_{xz}, d_{yz}\}$
- **Geometry**: Bilayer Kagome lattice of **Nb**.

Hamiltonian

$$
\begin{aligned}
H = & -t \sum_{\langle i,j\rangle,\sigma,\alpha} \left(c^{\dagger}_{i\sigma\alpha} c_{j\sigma\alpha} + \text{H.c.} \right) \\
& - t' \sum_{\langle\langle i,j\rangle\rangle,\sigma,\alpha} \left(c^{\dagger}_{i\sigma\alpha} c_{j\sigma\alpha} + \text{H.c.} \right) \\
& + U \sum_{i,\alpha} n^{d}_{i\uparrow\alpha} n^{d}_{i\downarrow\alpha} \\
& + V \sum_{\langle i,j\rangle,\sigma,\alpha} n_{i\sigma\alpha} n_{j\sigma\alpha}
\end{aligned}
$$

- **Extended Hubbard Model**
  1. NN Hopping terms: t.
  2. NNN Hopping terms: t'.
  3. Onsite interaction: U.
  4. NN interaction: U.
- **Convention**: $c_{i\sigma\alpha}$
  Annihilation operators of d_{α} orbitals at site i with spin σ.
  $\alpha \in \left\{ z^2; x^2 - y^2, xy; xz, yz \right\}$

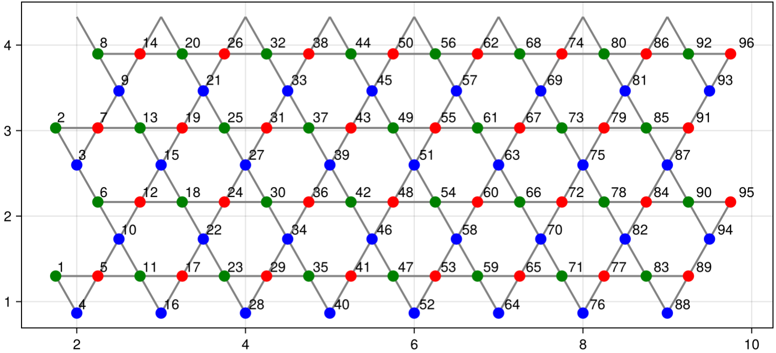
Hamiltonian

$$
\begin{aligned}
H = & - t_n \sum_{\langle i,j \rangle_n, \sigma, \alpha} \left(c^{\dagger}_{i\sigma\alpha} c_{j\sigma\alpha} + \text{H.c.} \right) \\
& + V_n \sum_{\langle i,j \rangle_n, \alpha} n_{i\sigma\alpha} n_{j\sigma\alpha}
\end{aligned}
$$

- **Extended Hubbard Model**
  1. n order neighbor hopping: t_n.
  2. n order neighbor interaction: V_n.
- **Convention**: $c_{i\sigma\alpha}$
  Annihilation operators of d_α orbitals at site i with spin σ.
  $\alpha \in \left\{ z^2; x^2 - y^2, xy; xz, yz \right\}$

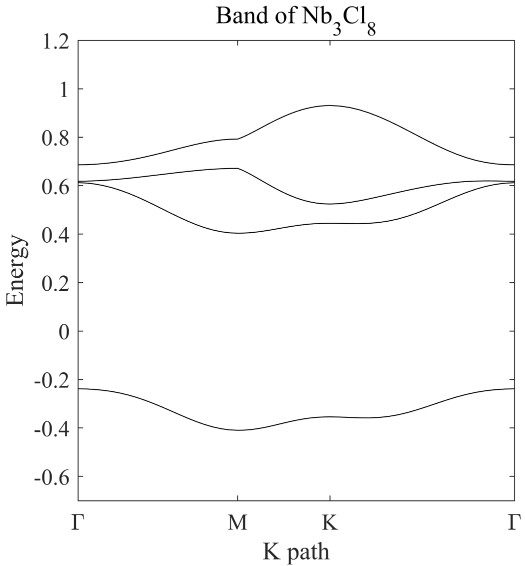
Parameters

- Composite Triangular Lattice ($Lx \times 4$ or 6) with **PBC**



- Parameters
  From DFT.

Observables



- some observables

  U1SU2: $n, n^d, \mathbf{S}_i \cdot \mathbf{S}_j,$ U1U1: $\cdots, S_z$

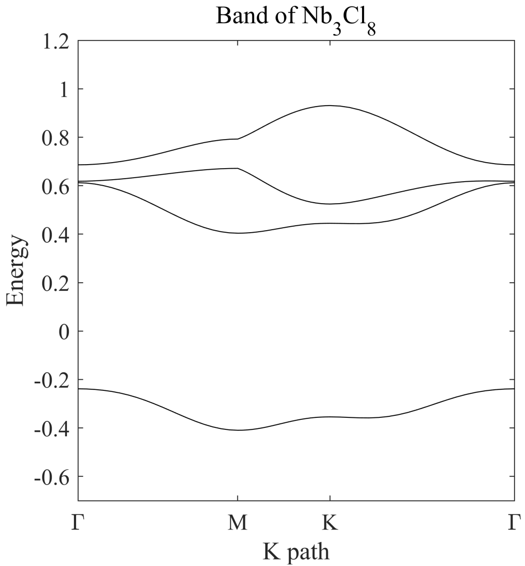
- Hamiltonian (Sing.Elec.Appr.)

$$H = \sum_{\mathbf{k},n,\sigma} E_n(\mathbf{k}) c^\dagger_{\mathbf{k}n\sigma} c_{\mathbf{k}n\sigma}$$

- CB breation operator $c^\dagger_{\mathbf{k}c\sigma}$

$$c^\dagger_{\mathbf{k}c\sigma} = \sum_{i,\alpha,\sigma} A_{c,i\alpha\sigma}(\mathbf{k}) \mathrm{e}^{i\mathbf{k}\cdot\mathbf{R}_i} c^\dagger_{i\alpha\sigma}$$

Observables



- Exciton pairing operator $\Delta^{\dagger}_{\mathbf{q}\beta}$

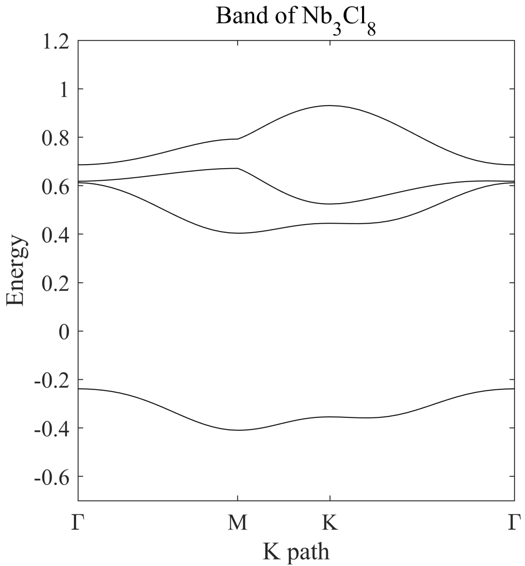
$$\Delta^{\dagger}_{\mathbf{k+q},\mathbf{k}S} = \frac{1}{\sqrt{2}}\left(c^{\dagger}_{\mathbf{k+q}c\uparrow}c_{\mathbf{k}v\downarrow} - c^{\dagger}_{\mathbf{k+q}c\downarrow}c_{\mathbf{k}v\uparrow}\right)$$

$$\Delta^{\dagger,0}_{\mathbf{k+q},\mathbf{k}T} = \frac{1}{\sqrt{2}}\left(c^{\dagger}_{\mathbf{k+q}c\uparrow}c_{\mathbf{k}v\downarrow} + c^{\dagger}_{\mathbf{k+q}c\downarrow}c_{\mathbf{k}v\uparrow}\right)$$

$$\Delta^{\dagger,1}_{\mathbf{k+q},\mathbf{k}T} = c^{\dagger}_{\mathbf{k+q}c\uparrow}c_{\mathbf{k}v\uparrow}$$

$$\Delta^{\dagger,-1}_{\mathbf{k+q},\mathbf{k}T} = c^{\dagger}_{\mathbf{k+q}c\downarrow}c_{\mathbf{k}v\downarrow}$$

Observables



- Properties $\Delta^{\dagger}_{\mathbf{k+q},\mathbf{k}\beta}$

$$\langle\Psi|\Delta_{\mathbf{k+q},\mathbf{k}\beta}|\Psi\rangle = 0$$
$$\langle\Psi|\Delta^{\dagger}_{\mathbf{k},\mathbf{k}'\beta}\Delta_{\bar{\mathbf{k}},\bar{\mathbf{k}}'\beta}|\Psi\rangle = ?$$

Observables

Definition

Triplet-pairing density matrix

$$\rho_T^z(\mathbf{k},\mathbf{k}';\bar{\mathbf{k}},\bar{\mathbf{k}}') = \left\langle \Delta^{\dagger,z}_{\mathbf{k},\mathbf{k}'T}\Delta^{z}_{\bar{\mathbf{k}},\bar{\mathbf{k}}'T} \right\rangle, \quad z = 0, 1, -1$$

Definition

Singlet-pairing density matrix

$$\rho_S(\mathbf{k},\mathbf{k}';\bar{\mathbf{k}},\bar{\mathbf{k}}') = \left\langle \Delta^{\dagger}_{\mathbf{k},\mathbf{k}'S}\Delta_{\bar{\mathbf{k}},\bar{\mathbf{k}}'S} \right\rangle$$

Observables

Definition

$\mathbf{k}$ space pairing operator

$$\Delta_{\mathbf{k},\mathbf{k}'} = c^{\dagger}_{\mathbf{k}c} c_{\mathbf{k}'v} = \sum_{s,l} c^{\dagger}_{s} c_{l} A^{*}_{c,i}(\mathbf{k}) A_{v,j}(\mathbf{k}') \mathrm{e}^{i(\mathbf{k}\cdot\mathbf{R}_s - \mathbf{k}'\cdot\mathbf{R}_l)}$$

Definition

real space pairing operator

$$\begin{aligned}
\Delta_{\mathbf{i},\mathbf{j}} &= \int_{\mathbf{k},\mathbf{k}'} \Delta_{\mathbf{k},\mathbf{k}'} \mathrm{e}^{i(-\mathbf{k}\cdot\mathbf{R}_i + \mathbf{k}'\cdot\mathbf{R}_j)} \\
&= \sum_{s,l} c^{\dagger}_{s} c_{l} \int_{\mathbf{k},\mathbf{k}'} A^{*}_{c,i}(\mathbf{k}) A_{v,j}(\mathbf{k}') \mathrm{e}^{i(\mathbf{k}\cdot\mathbf{R}_s - \mathbf{k}'\cdot\mathbf{R}_l)} \mathrm{e}^{i(-\mathbf{k}\cdot\mathbf{R}_i + \mathbf{k}'\cdot\mathbf{R}_j)}
\end{aligned}$$

PROBLEMS

- real-space pairing operator do not exists
- Calculate 2-PBC system, which more close to a lattice system. 1-PBC for a stripe.