## BrillouinZone

### August 5, 2018

# Information about the first Brillouin zone for generalized triangle lattice

#### 1.1 Translation vectors of real space

- $\mathbf{a}_0 = (1,0)$
- $\mathbf{a}_1 = (\frac{1}{2}, \frac{\sqrt{3}}{2})$

### 1.2 Translation vectors of reciprocal space

- $\mathbf{b}_0 = (2\pi, -\frac{2\pi}{\sqrt{3}})$   $\mathbf{b}_1 = (0, \frac{4\pi}{\sqrt{3}})$

### 1.3 $\Gamma$ point

•  $\Gamma = (0,0)$ 

## 1.4 M points

- $M_0 = (-\pi, \frac{\pi}{\sqrt{3}})$

- $M_1 = (0, \frac{2\pi}{\sqrt{3}})$   $M_2 = (\pi, \frac{\pi}{\sqrt{3}})$   $M_3 = (\pi, -\frac{\pi}{\sqrt{3}})$   $M_4 = (0, -\frac{2\pi}{\sqrt{3}})$   $M_5 = (-\pi, -\frac{\pi}{\sqrt{3}})$

## 1.5 K points

- $K_0 = \left(-\frac{4\pi}{3}, 0\right)$   $K_1 = \left(-\frac{2\pi}{3}, \frac{2\pi}{\sqrt{3}}\right)$
- $K_2 = (\frac{2\pi}{3}, \frac{2\pi}{\sqrt{3}})^{\frac{1}{3}}$

- $K_3 = (\frac{4\pi}{3}, 0)$   $K_4 = (\frac{2\pi}{3}, -\frac{2\pi}{\sqrt{3}})$   $K_5 = (-\frac{2\pi}{3}, -\frac{2\pi}{\sqrt{3}})$

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In [1]: from itertools import product
        import matplotlib.pyplot as plt
        import numpy as np
In [2]: dx = dy = 0.3
        dtype = np.float64
        # Translation vectors of real space and reciprocal space
        As = np.array([[1.0, 0.0], [0.5, np.sqrt(3)/2]], dtype=dtype)
        Bs = 2 * np.pi * np.array([[1.0, -1/np.sqrt(3)], [0.0, 2/np.sqrt(3)]], dtype=dtype)
        # Some high symmetry points in the first Brillouin zone
        Gamma = np.array([0.0, 0.0], dtype=dtype)
        Ks = 2 * np.pi * np.array(
            [[-2/3.0, 0.0], [-1/3.0, 1/np.sqrt(3)], [1/3.0, 1/np.sqrt(3)],
             [2/3.0, 0.0], [1/3.0, -1/np.sqrt(3)], [-1/3.0, -1/np.sqrt(3)]],
            dtype=dtype
        )
        Ms = np.pi * np.array(
            [[-1.0, 1/np.sqrt(3)], [0.0, 2/np.sqrt(3)], [1.0, 1/np.sqrt(3)],
             [1.0, -1/\text{np.sqrt}(3)], [0.0, -2/\text{np.sqrt}(3)], [-1.0, -1/\text{np.sqrt}(3)]],
            dtype=dtype
        )
        fig, ax = plt.subplots()
        fig.set_size_inches(w=16, h=9)
        ax.set_aspect("equal")
        ax.set_axis_off()
        # Draw the boundary of the first Brillouin zone
        color0 = "#6C71C4"
        color1 = "#F57900"
        for config in product(range(-1, 2), repeat=2):
            K = np.matmul(config, Bs)
            ax.plot(K[0], K[1], marker="o", mec=color0, mfc=color0, markersize=8)
            ax.text(K[0]+dx, K[1]-dy, str(config), size="large", color=color0)
            if config !=(0, 0):
                center = K / 2
                orthogonal_vector = np.array([-K[1], K[0]])
                p0 = center + orthogonal_vector
                p1 = center - orthogonal_vector
                ax.plot((p0[0], p1[0]), (p0[1], p1[1]), color=color1, lw=2)
        size = "xx-large"
```

```
# Draw the Gamma point
color = "#EF2929"
ax.plot(Gamma[0], Gamma[1], marker='o', mec=color, mfc=color, markersize=12)
    Gamma[0]+dx, Gamma[1]+dy, s=r"$\mathit{\Gamma}$",
    size=size, color=color
)
# Draw the M points
color = "#3465A4"
for x, y in Ms:
    ax.plot(x, y, marker='o', mec=color, mfc=color, markersize=12)
    ax.text(x+dx, y+dy, s=r"$\mathit{M}$", size=size, color=color)
# Draw the K points
color= "#5C3566"
for x, y in Ks:
    ax.plot(x, y, marker='o', mec=color, mfc=color, markersize=12)
    ax.text(x+dx, y+dy, s=r"$\mathit{K}$", size=size, color=color)
plt.show()
```

