Plotting 2D band structure images in Cartesian space in PythTB

Christopher Gutiérrez

27 December 2019

In the Python-based tight-binding code PythTB[1], the default method for inputting the reciprocal space k-vectors for calculating eigenvalues and eigenvectors is in the basis of the reciprocal lattice vectors, $\mathbf{b}_i$. That is,

$$\mathbf{k} = \gamma_1 \mathbf{b}_1 + \gamma_2 \mathbf{b}_2 + \gamma_3 \mathbf{b}_3, \tag{1}$$

where $\gamma_i \in \mathbb{R}$ are dimensionless real numbers that are provided by the user. One thus inputs the k-grid of γ_is that the tight-binding (TB) model is to be solved over. While this provides a very clear and simple way to calculate 1-D band structure (*i.e.* "spaghetti") plots along high-symmetry directions, it can lead to distorted images when plotting 2-D band structures for crystals with non-square symmetries (Fig. 1). In this Python code snippet I show how one can instead input a set of γ_is such that the k-mesh is in the Cartesian basis

$$\mathbf{k} = k_x \hat{x} + k_y \hat{y} + k_z \hat{z}, \tag{2}$$

where $k_i \in \mathbb{R}$ have units of the reciprocal lattice (*i.e.* Å^{-1}) in Cartesian space. While this necessarily is more computationally costly, since redundant points outside of the first Brillouin zone (BZ) are calculated, it provides nice 2-D images without having to perform any image post-processing, such as an affine transformation.

Here, I provide the mathematical derivation that will provide us the proper set of γ_is that will describe a Cartesian k-mesh:

Firstly, given a set of direct crystal lattice vectors $\mathbf{a}_i$, there is a set of reciprocal lattice vectors that, *by definition*, satisfy

$$\mathbf{a}_i \cdot \mathbf{b}_j = 2\pi \delta_{ij}, \tag{3}$$

where $i, j = 1, 2, 3$ enumerate the vectors that describe a three-dimensional crystal and δ_{ij} is the Kronecker delta. It will be instructive later to write Eq. 3 in a compact matrix form. To do this, let's express $\mathbf{a}_i, \mathbf{b_j}$ in Cartesian basis:

$$\mathbf{a}_i = \alpha_{i1} \hat{x} + \alpha_{i2} \hat{y} + \alpha_{i3} \hat{z} \tag{4}$$

$$\mathbf{b}_j = \beta_{j1} \hat{x} + \beta_{j2} \hat{y} + \beta_{j3} \hat{z}, \tag{5}$$

where α_{ij}, β_{ij} are real-valued numbers in real and reciprocal space, respectively, and the second indices correspond to vector components. This allows to re-write the dot product in

[1] http://physics.rutgers.edu/pythtb/index.html; S. Coh, D. Vanderbilt, Python Tight Binding (PythTB) (2013).

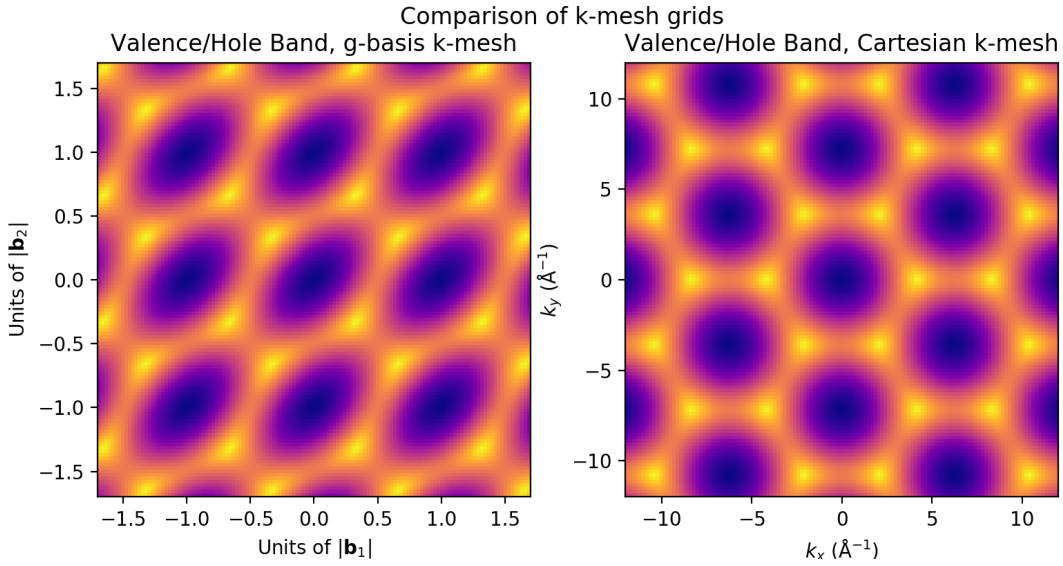

Figure 1: **Two-dimensional band structure calculations.** *Left:* False-color image of energy eigenvalues calculated over a k-mesh grid in the basis of the reciprocal lattice vectors $\mathbf{b}_1, \mathbf{b}_2$. *Right:* Same as left panel, except calculated over a Cartesian k-mesh grid.

Eq. 3 as a product of matrices

$$\underbrace{\begin{pmatrix} \alpha_{11} & \alpha_{12} & \alpha_{13} \\ \alpha_{21} & \alpha_{22} & \alpha_{23} \\ \alpha_{31} & \alpha_{32} & \alpha_{33} \end{pmatrix}}_{\mathbf{A}} \underbrace{\begin{pmatrix} \beta_{11} & \beta_{21} & \beta_{31} \\ \beta_{12} & \beta_{22} & \beta_{32} \\ \beta_{13} & \beta_{23} & \beta_{33} \end{pmatrix}}_{\mathbf{B}^\top} = 2\pi \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \tag{6}$$

where $\mathbf{B}^\top$ is the matrix transpose of $\mathbf{B}$. The coefficients α_{ij}, β_{ij} that describe the real and reciprocal lattice vectors are related by

$$\mathbf{A} = 2\pi \left\{\mathbf{B}^\top\right\}^{-1} \tag{7}$$

$$\begin{pmatrix} \alpha_{11} & \alpha_{12} & \alpha_{13} \\ \alpha_{21} & \alpha_{22} & \alpha_{23} \\ \alpha_{31} & \alpha_{32} & \alpha_{33} \end{pmatrix} = 2\pi \begin{pmatrix} \beta_{11} & \beta_{21} & \beta_{31} \\ \beta_{12} & \beta_{22} & \beta_{32} \\ \beta_{13} & \beta_{23} & \beta_{33} \end{pmatrix}^{-1}. \tag{8}$$

Note that the inverse matrices exist since both the direct and reciprocal crystal lattice vectors are linearly independent. As an aside, it's neat to instead solve for $\mathbf{B}$,

$$\mathbf{B} = 2\pi \left\{\mathbf{A}^\top\right\}^{-1} \tag{9}$$

$$\begin{pmatrix} \beta_{11} & \beta_{12} & \beta_{13} \\ \beta_{21} & \beta_{22} & \beta_{23} \\ \beta_{31} & \beta_{32} & \beta_{33} \end{pmatrix} = 2\pi \begin{pmatrix} \alpha_{11} & \alpha_{21} & \alpha_{31} \\ \alpha_{12} & \alpha_{22} & \alpha_{32} \\ \alpha_{13} & \alpha_{23} & \alpha_{33} \end{pmatrix}^{-1}, \tag{10}$$

whence one can see that the inverse matrix of $\mathbf{A}^\top$ agrees with the well-known definition of the reciprocal lattice vectors, *e.g.*

$$\mathbf{b}_1 = 2\pi \frac{\mathbf{a}_2 \times \mathbf{a}_3}{|\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)|} \tag{11}$$

and the triple-product in the denominator corresponds to the determinant of $\mathbf{A}$ in Eq. 10.

We are now ready to find the set of (γ_1,γ_2,γ_3) values that will describe an evenly-spaced Cartesian grid of points (k_x, k_y, k_z). To find these γ_is we expand Eq. 1 in Cartesian basis:

$$\mathbf{k} = \gamma_1\mathbf{b}_1 + \gamma_2\mathbf{b}_2 + \gamma_3\mathbf{b}_3 \tag{12}$$

$$\mathbf{k} = \gamma_1(\beta_{11}\hat{x} + \beta_{12}\hat{y} + \beta_{13}\hat{z}) + \gamma_2(\beta_{21}\hat{x} + \beta_{22}\hat{y} + \beta_{23}\hat{z}) + \gamma_3(\beta_{31}\hat{x} + \beta_{32}\hat{y} + \beta_{33}\hat{z}) \tag{13}$$

$$\mathbf{k} = (\gamma_1\beta_{11} + \gamma_2\beta_{21} + \gamma_3\beta_{31})\hat{x} + (\gamma_1\beta_{12} + \gamma_2\beta_{22} + \gamma_3\beta_{32})\hat{y} + (\gamma_1\beta_{13} + \gamma_2\beta_{23} + \gamma_3\beta_{33})\hat{z}. \tag{14}$$

Matching each Cartesian component of Eq. 2 with Eq. 14 yields a matrix relation between the γ_is and k_is:

$$\begin{pmatrix} k_x \\ k_y \\ k_z \end{pmatrix} = \underbrace{\begin{pmatrix} \beta_{11} & \beta_{21} & \beta_{31} \\ \beta_{12} & \beta_{22} & \beta_{32} \\ \beta_{13} & \beta_{23} & \beta_{33} \end{pmatrix}}_{\mathbf{B}^\top} \begin{pmatrix} \gamma_1 \\ \gamma_2 \\ \gamma_3 \end{pmatrix} \tag{15}$$

$$\mathbf{k} = \mathbf{B}^\top \cdot \boldsymbol{\gamma} \tag{16}$$

Multiplying on the left by $\left\{\mathbf{B}^\top\right\}^{-1}$ and using Eq. 7 we finally arrive at

$$\boxed{\begin{pmatrix} \gamma_1 \\ \gamma_2 \\ \gamma_3 \end{pmatrix} = \frac{1}{2\pi} \underbrace{\begin{pmatrix} \alpha_{11} & \alpha_{12} & \alpha_{13} \\ \alpha_{21} & \alpha_{22} & \alpha_{23} \\ \alpha_{31} & \alpha_{32} & \alpha_{33} \end{pmatrix}}_{\mathbf{A}} \begin{pmatrix} k_x \\ k_y \\ k_z \end{pmatrix}} \tag{17}$$

$$\boldsymbol{\gamma} = \frac{1}{2\pi}\mathbf{A} \cdot \mathbf{k}. \tag{18}$$

Thus, given a user's desired mesh grid of k points with dimensions (k_x, k_y, k_z) (in units of reciprocal lattice, Å^{-1}) one inputs the $(\gamma_1, \gamma_2, \gamma_3)$ given by the above.