Siesta Band Unfolding Document

A manual for the BUFDeepH code.

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Contents

Here is one band unfolding method to transfer from the deeph-format Hamitonian data to a unfolded band structure. This code is for two-dimensional Moire honeycomb lattice. For other cases, only minor modifications are needed.

Section 1: Band unfolding method

Hamilton basis:

$$\langle \boldsymbol{r}|\alpha, \boldsymbol{k}\rangle = \frac{1}{\sqrt{N}}\sum_{\boldsymbol{R}} e^{i\boldsymbol{k}\cdot\boldsymbol{R}}\phi(\boldsymbol{r}-\boldsymbol{R}-\boldsymbol{\tau}_\alpha) \qquad [1]$$

Bloch wfc:

$$\begin{aligned}|n, \boldsymbol{k}\rangle &= \sum_{\alpha}\varphi_{n\alpha}(\boldsymbol{k})|\alpha, \boldsymbol{k}\rangle \\ \langle \boldsymbol{r}|n, \boldsymbol{k}\rangle &= \frac{1}{\sqrt{N}}\sum_{\alpha,\boldsymbol{R}} e^{i\boldsymbol{k}\cdot\boldsymbol{R}}\phi(\boldsymbol{r}-\boldsymbol{R}-\boldsymbol{\tau}_\alpha)\varphi_{n\alpha}(\boldsymbol{k})\end{aligned} \qquad [2]$$

Define

$$\phi(\boldsymbol{p}) = \int d^3\boldsymbol{r} e^{-i\boldsymbol{p}\cdot(\boldsymbol{r}-\boldsymbol{R}-\boldsymbol{\tau}_\alpha)}\phi(\boldsymbol{r}-\boldsymbol{R}-\boldsymbol{\tau}_\alpha) \qquad [3]$$

as the Fourier transform of $\phi(\boldsymbol{r})$, then

$$\begin{aligned}\langle \boldsymbol{p}|n, \boldsymbol{k}\rangle &= \frac{1}{N}\sum_{\alpha,R}\int d^3\boldsymbol{r} e^{-i\boldsymbol{p}\cdot\boldsymbol{r}}e^{i\boldsymbol{k}\cdot\boldsymbol{R}}\phi(\boldsymbol{r}-\boldsymbol{R}-\boldsymbol{\tau}_\alpha)\varphi_{n\alpha}(\boldsymbol{k}) \\ &= \frac{1}{N}\sum_{\alpha,\boldsymbol{R}} e^{i(\boldsymbol{k}-\boldsymbol{p})\cdot\boldsymbol{R}}e^{-i\boldsymbol{p}\cdot\boldsymbol{\tau}_\alpha}\phi(\boldsymbol{p})\varphi_{n\alpha}(\boldsymbol{k}) \\ &= \sum_{\alpha,\boldsymbol{G}}\delta_{\boldsymbol{p}_{||},\boldsymbol{k}+\boldsymbol{G}}e^{-i\boldsymbol{p}\cdot\boldsymbol{\tau}_\alpha}\phi(\boldsymbol{p})\varphi_{n\alpha}(\boldsymbol{k})\end{aligned} \qquad [4]$$

For ARPES, the intensity is given by

$$\begin{aligned}I(\boldsymbol{p}, E) &\propto \sum_{n,\boldsymbol{k}}|\langle \boldsymbol{p}|\boldsymbol{A}\cdot\hat{\boldsymbol{v}}|n, \boldsymbol{k}\rangle|^2\ \delta(E-\varepsilon_{n\boldsymbol{k}}) \\ &= \sum_{n,\boldsymbol{k}}|\boldsymbol{A}\cdot\sum_{\alpha,\beta,\boldsymbol{k}'}\langle \boldsymbol{p}|\alpha, \boldsymbol{k}'\rangle\langle\alpha, \boldsymbol{k}'|\hat{\boldsymbol{v}}|\beta, \boldsymbol{k}'\rangle\langle\beta, \boldsymbol{k}'|n, \boldsymbol{k}\rangle|^2\ \delta(E-\varepsilon_{n\boldsymbol{k}}) \\ &= |\phi(\boldsymbol{p})|^2\sum_{n,\boldsymbol{k}}|\boldsymbol{A}\cdot\sum_{\alpha,\beta,\boldsymbol{G}}\delta_{\boldsymbol{p}_{||},\boldsymbol{k}+\boldsymbol{G}}e^{-i\boldsymbol{p}\cdot\boldsymbol{\tau}_\alpha}\langle\alpha, \boldsymbol{k}|\partial_{\boldsymbol{k}}\hat{H}|\beta, \boldsymbol{k}\rangle\varphi_{n\beta}(\boldsymbol{k})|^2\ \delta(E-\varepsilon_{n\boldsymbol{k}}) \\ or &= |\phi(\boldsymbol{p})|^2\sum_{n,\boldsymbol{k},\alpha}|(\boldsymbol{A}\cdot\boldsymbol{p})^2\delta_{\boldsymbol{p}_{||},\boldsymbol{k}+\boldsymbol{G}}e^{-i\boldsymbol{p}\cdot\boldsymbol{\tau}_\alpha}\varphi_{n\beta}(\boldsymbol{k})|^2\ \delta(E-\varepsilon_{n\boldsymbol{k}})\end{aligned} \qquad [5]$$

To simplify the problem, we regard the real spherical harmonic basis as the delta function.

For unfolding, similarly, we have

$$\begin{aligned} I(\boldsymbol{p}, E) &\propto \sum_{g} \sum_{N,\boldsymbol{K}} |\langle \boldsymbol{p}+\boldsymbol{g}|N,\boldsymbol{K}\rangle|^2 \ \delta(E-\varepsilon_{N\boldsymbol{K}}) \\ &= |\phi(\boldsymbol{p})|^2 \sum_{g,N,\boldsymbol{K},\alpha,G} |\delta_{\boldsymbol{p}+\boldsymbol{g},\boldsymbol{K}+\boldsymbol{G}} e^{-i(\boldsymbol{p}+\boldsymbol{g})\cdot\boldsymbol{\tau}_\alpha} \varphi_{N\alpha}(\boldsymbol{K})|^2 \ \delta(E-\varepsilon_{N\boldsymbol{K}}) \end{aligned} \quad [6]$$

where capital letters for moire cell and small letters for primitive cell.

Section 2: Unfolding Steps

Back to eq.6, in fact, we project the Bloch wave function using a set of plane waves. From the perspective of band folding, the bands at det(M) G-points in a pBZ are all folded into an mBZ. Conversely, we only need to distinguish which G-point each band comes from, that is, to look at the weight with the largest projection component.

Step1 For each p in the KPATH, find $p = K + G_0$, where K in the (0,0)'s mBZ.

Step2 For the K given in the Step1, find all $k = K + G_m$, where $m = 1, 2, ..., \det(M)$.

Step3 For each k given in the Step2, calculate weight w_m and save maximum $\max(w_m)$.

Step4 Compare $\max(w_m)$ with w_0 in Step1, if w_0 is maximum, then accept this unfolding action.