Wannier Functions

(Technique Details of *Wannier90*)

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Definition of $\widehat{T}_l$

For crystal system, the Hamiltonian commutes with the translation operators $\widehat{T}_l$.

$$\left[\widehat{T}_l, \widehat{H}\right] = 0 \tag{1}$$

Where $\widehat{H} = \widehat{T} + \widehat{V}(\mathbf{r})$, $\widehat{V}(\mathbf{r}) = \widehat{V}(\mathbf{r} + \mathbf{R}_l)$, $\widehat{T}_l|\psi(\mathbf{r})\rangle = |\psi(\mathbf{r} + \mathbf{R}_l)\rangle$, $\mathbf{R}_l = \sum_{i=1}^{3} l_i \mathbf{a}_i$, and $\{\mathbf{a}_i\}$ is the lattice vector.

Properties

$$\left.\begin{aligned} \widehat{T}_l \widehat{T}_{l'} &= \widehat{T}_{l+l'} \\ \widehat{T}_l|\psi(\mathbf{r})\rangle &= t_l|\psi(\mathbf{r})\rangle \end{aligned}\right\} \Rightarrow t_{l+l'} = t_l \cdot t_{l'}$$

The eigenvalue of $\widehat{T}_l$ can be written as:

$$t_l = (t_{\mathbf{a}_1})^{l_1} (t_{\mathbf{a}_2})^{l_2} (t_{\mathbf{a}_3})^{l_3} \tag{2}$$

Eigenvalue of $\widehat{T}_l$

Let $\widehat{T}(\mathbf{a}_i)|\psi(\mathbf{r})\rangle = |\psi(\mathbf{r}+l_i\mathbf{a}_i)\rangle$. The translation operator $\widehat{T}(\mathbf{a}_i)$ generates a cyclic group C_{N_i} in the real space, where N_i is the cell quantity in $\mathbf{a}_i$ direction among one period of total wave functions.

Noting

Since the C_{N_i} is also a finite ablian group, according to *Schur's Lemma I*, all of its irreducible unitary representation is one dimensional, which means, $t(\mathbf{a}_i) = \mathrm{e}^{\mathrm{i}2\pi y_i}$

Using the periodic conditions: $t(\mathbf{a}_i)^{N_i} = 1$, one can easily conclude that,

$$t(\mathbf{a}_i) = \mathrm{e}^{\mathrm{i}2\pi\frac{m_i}{N_i}} \tag{3a}$$

$$t_l = \mathrm{e}^{\mathrm{i}2\pi\left(\frac{m_1 l_1}{N_1}+\frac{m_2 l_2}{N_2}+\frac{m_3 l_3}{N_3}\right)} \tag{3b}$$

If we set $\mathbf{k} = \frac{m_1}{N_1}\mathbf{b}_1 + \frac{m_2}{N_2}\mathbf{b}_2 + \frac{m_3}{N_3}\mathbf{b}_3$, and $\mathbf{a}_i \cdot \mathbf{b}_j = 2\pi\delta_{ij}$

Bloch Theorem

If we set $\mathbf{k} = \frac{m_1}{N_1}\mathbf{b}_1 + \frac{m_2}{N_2}\mathbf{b}_2 + \frac{m_3}{N_3}\mathbf{b}_3$, and $\mathbf{a}_i \cdot \mathbf{b}_j = 2\pi\delta_{ij}$
Then the expression of t_l can be rewritten as:

$$t_l = \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{R}_l} \tag{4}$$

The operators set: $\{\widehat{H}, \widehat{T}_1, \widehat{T}_2, ..., \widehat{T}_l, ...\}$ constitute the CSCO of the crystal system, which means the eigenstate of $\widehat{H}$ can also be the eigenstate of $\widehat{T}_l$.

$$\widehat{T}_l \left|\psi_n^{\mathbf{k}}(\mathbf{r})\right\rangle = \left|\psi_n^{\mathbf{k}}(\mathbf{r}+\mathbf{R}_l)\right\rangle = \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{R}_l}\left|\psi_n^{\mathbf{k}}(\mathbf{r})\right\rangle \tag{5}$$

Bloch Theorem (in rough language)

Let $\left|\psi_n^{\mathbf{k}}(\mathbf{r})\right\rangle = \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}}\left|u_n^{\mathbf{k}}(\mathbf{r})\right\rangle$, and set $\left|u_n^{\mathbf{k}}(\mathbf{r})\right\rangle = \left|u_n^{\mathbf{k}}(\mathbf{r}+\mathbf{R}_l)\right\rangle$. Then the expression (5) will be satisfied automatically. (We found a formal solution for the Hamiltonian under a periodic system.)

A Key Property

Bloch Theorem (more specifically)

If the Hamiltonian of the system $\widehat{H} = \widehat{T} + \widehat{V}(\mathbf{r})$ satisfies,

$$V(\mathbf{r}) = V(\mathbf{r} + \mathbf{R}_l)$$

Then the wave functions of such a system can be written as,

$$\left|\psi_n^{\mathbf{k}}(\mathbf{r})\right\rangle = \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}} \left|u_n^{\mathbf{k}}(\mathbf{r})\right\rangle$$

Where $\left|u_n^{\mathbf{k}}(\mathbf{r})\right\rangle = \left|u_n^{\mathbf{k}}(\mathbf{r} + \mathbf{R}_l)\right\rangle$, $\mathbf{k} = \sum_{i=1}^{3} \frac{m_i}{N_i}\mathbf{b}_i$, $\mathbf{R}_l = \sum_{i=1}^{3} l_i \mathbf{a}_i$, $\mathbf{a}_i \cdot \mathbf{b}_j = 2\pi\delta_{ij}$.

The Key Property

Adding a arbitrary phase $\phi_n(\mathbf{k})$ to the bloch wave, $\psi_n^{\mathbf{k}(\mathbf{r})} \to \tilde{\psi}_n^{\mathbf{k}(\mathbf{r})} = \psi_n^{\mathbf{k}(\mathbf{r})}\mathrm{e}^{\mathrm{i}\phi_n(\mathbf{k})}$, will not break the derivation above. Typically, $\psi_n^{\mathbf{k}(\mathbf{r})} \to \tilde{\psi}_n^{\mathbf{k}(\mathbf{r})}$ is called a "gauge transformation". (This is the very important property we must understand before the Wannier functions' discussion.)

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Definition

Wannier Functions

Wannier functions are Fourier transforms of the Bloch eigenstate. For one band i the function associated with the cell labeled by lattice point $\mathbf{R}_m$ is,

$$\begin{aligned} \left| w_i^{\mathbf{R}_m} \right\rangle &= \frac{V}{(2\pi)^3} \int_{BZ} d^3k \, \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{R}_m} \left| \psi_i^{\mathbf{k}} \right\rangle \\ &= \frac{V}{(2\pi)^3} \int_{BZ} d^3k \, \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot(\mathbf{r}-\mathbf{R}_m)} \left| u_i^{\mathbf{k}} \right\rangle \end{aligned} \tag{6}$$

Also, we can write the formulas in terms of discrete sums:

$$\left| w_i^{\mathbf{R}_m} \right\rangle = \frac{1}{N_{\mathbf{k}}} \sum_{\mathbf{k}} \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot(\mathbf{r}-\mathbf{R}_m)} \left| u_i^{\mathbf{k}} \right\rangle \tag{7}$$

Orthogonality of Wannier Functions

$$\left\langle w_i^{\mathbf{R}_m} \middle| w_j^{\mathbf{R}_n} \right\rangle = \left[\frac{V}{(2\pi)^3}\right]^2 \int_{BZ} d^3k \int_{BZ} d^3k' \mathrm{e}^{-\mathrm{i}\mathbf{k}'\cdot(\mathbf{r}-\mathbf{R}_m)} \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot(\mathbf{r}-\mathbf{R}_n)} \left\langle u_i^{\mathbf{R}_m} \middle| u_j^{\mathbf{R}_n} \right\rangle$$
$$= \frac{V}{(2\pi)^3}\delta_{ij}\delta_{mn} \tag{8}$$

Inverse Transformation

We can also represent the Bloch wave functions using Wannier functions by the expression:

$$\left|\psi_i^{\mathbf{k}}\right\rangle = \sum_m \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{R}_m} \left| w_i^{\mathbf{R}_m} \right\rangle \tag{9}$$

Small Exercise

Exercise

Now, try to calculate the two expressions listed below.

$$\left\langle w_i^{\mathbf{R}} \middle| \widehat{\mathbf{r}} \middle| w_j^{\mathbf{0}} \right\rangle \tag{10a}$$

$$\left\langle w_i^{\mathbf{R}} \middle| \widehat{\mathbf{r}}^2 \middle| w_j^{\mathbf{0}} \right\rangle \tag{10b}$$

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$$\left\langle w_i^{\mathbf{R}} \middle| \widehat{\mathbf{r}} \middle| w_j^{\mathbf{0}} \right\rangle \tag{10a}$$

$$\left\langle w_i^{\mathbf{R}} \middle| \widehat{\mathbf{r}}^2 \middle| w_j^{\mathbf{0}} \right\rangle \tag{10b}$$

Solution

$$\begin{aligned}
\left\langle u_i^{\mathbf{k}} \middle| u_j^{\mathbf{k}+\mathbf{q}} \right\rangle &= \left\langle \psi_i^{\mathbf{k}} \middle| \mathrm{e}^{-\mathrm{i}\mathbf{q}\cdot\mathbf{r}} \middle| \psi_j^{\mathbf{k}+\mathbf{q}} \right\rangle \\
&= \sum_{mn} \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot(\mathbf{R}_m-\mathbf{R}_n)} \left\langle w_i^{\mathbf{R}_m} \middle| \mathrm{e}^{-\mathrm{i}\mathbf{q}\cdot\mathbf{r}} \middle| w_j^{\mathbf{R}_n} \right\rangle \\
&= \sum_{\mathbf{R}} \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{R}} \left\langle w_i^{\mathbf{R}} \middle| \mathrm{e}^{-\mathrm{i}\mathbf{q}\cdot\mathbf{r}} \middle| w_j^{\mathbf{0}} \right\rangle, \quad (\mathbf{R} = \mathbf{R}_m - \mathbf{R}_n)
\end{aligned}$$

where $\mathbf{q}$ are vectors much less than $\mathbf{k}$.

Small Exercise

Solution

$$\left\langle u_i^{\mathbf{k}} \middle| u_j^{\mathbf{k}+\mathbf{q}} \right\rangle = \sum_{\mathbf{R}} \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{R}} \left\langle w_i^{\mathbf{R}} \middle| \mathrm{e}^{-\mathrm{i}\mathbf{q}\cdot\mathbf{r}} \middle| w_j^{\mathbf{0}} \right\rangle$$

By using Taylor expansion,

$$\left| u_j^{\mathbf{k}+\mathbf{q}} \right\rangle = \left| u_j^{\mathbf{k}} \right\rangle + \nabla_{\mathbf{k}} \left| u_j^{\mathbf{k}} \right\rangle \cdot \mathbf{q} + \frac{1}{2} \nabla_{\mathbf{k}}^2 \left| u_j^{\mathbf{k}} \right\rangle \cdot \mathbf{q}^2 + \dots$$

$$\mathrm{e}^{-\mathrm{i}\mathbf{q}\cdot\mathbf{r}} = 1 - \mathrm{i}\mathbf{r}\cdot\mathbf{q} - \frac{1}{2}\mathbf{r}^2\mathbf{q}^2$$

Comparing the order of $\mathbf{q}$, we finally get,

$$\left\langle u_i^{\mathbf{k}} \middle| \nabla_{\mathbf{k}} \middle| u_j^{\mathbf{k}} \right\rangle = \sum_{\mathbf{k}} \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{R}} \left\langle w_i^{\mathbf{R}} \middle| -i\mathbf{r} \middle| w_j^{\mathbf{0}} \right\rangle \tag{11a}$$

$$\left\langle w_i^{\mathbf{R}} \middle| \mathbf{r} \middle| w_j^{\mathbf{0}} \right\rangle = \mathrm{i} \frac{V}{(2\pi)^3} \int_{BZ} d^3k \, \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{R}} \left\langle u_i^{\mathbf{k}} \middle| \nabla_{\mathbf{k}} \middle| u_j^{\mathbf{k}} \right\rangle \tag{11b}$$

Small Exercise

Solution

Similarly,

$$\left\langle u_i^{\mathbf{k}} \middle| \nabla_{\mathbf{k}}^2 \middle| u_j^{\mathbf{k}} \right\rangle = \sum_{\mathbf{k}} \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{R}} \left\langle w_i^{\mathbf{R}} \middle| -\mathbf{r}^2 \middle| w_j^{\mathbf{0}} \right\rangle \tag{12a}$$

$$\left\langle w_i^{\mathbf{R}} \middle| \mathbf{r}^2 \middle| w_j^{\mathbf{0}} \right\rangle = -\frac{V}{(2\pi)^3} \int_{BZ} d^3k \, \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{R}} \left\langle u_i^{\mathbf{k}} \middle| \nabla_{\mathbf{k}}^2 \middle| u_j^{\mathbf{k}} \right\rangle \tag{12b}$$

In conclusion,

$$\left\langle w_i^{\mathbf{R}} \middle| \mathbf{r} \middle| w_j^{\mathbf{0}} \right\rangle = \mathrm{i}\frac{V}{(2\pi)^3} \int_{BZ} d^3k \, \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{R}} \left\langle u_i^{\mathbf{k}} \middle| \nabla_{\mathbf{k}} \middle| u_j^{\mathbf{k}} \right\rangle$$

$$\left\langle w_i^{\mathbf{R}} \middle| \mathbf{r}^2 \middle| w_j^{\mathbf{0}} \right\rangle = -\frac{V}{(2\pi)^3} \int_{BZ} d^3k \, \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{R}} \left\langle u_i^{\mathbf{k}} \middle| \nabla_{\mathbf{k}}^2 \middle| u_j^{\mathbf{k}} \right\rangle$$

"Problem" of Wannier Functions

Noting

The most serious drawback of the Wannier representation is that the functions are not uniquely defined.

$$\left|w_i^{\mathbf{R}_m}\right\rangle = \frac{V}{(2\pi)^3}\int_{BZ} d^3k\ \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot(\mathbf{r}-\mathbf{R}_m)}\left|u_i^{\mathbf{k}}\right\rangle$$

$$\left|\tilde{w}_i^{\mathbf{R}_m}\right\rangle = \frac{V}{(2\pi)^3}\int_{BZ} d^3k\ \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot(\mathbf{r}-\mathbf{R}_m)}\left|\tilde{u}_i^{\mathbf{k}}\right\rangle$$

$$= \frac{V}{(2\pi)^3}\int_{BZ} d^3k\ \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot(\mathbf{r}-\mathbf{R}_m)}\mathrm{e}^{\mathrm{i}\phi_i^{\mathbf{k}}}\left|u_i^{\mathbf{k}}\right\rangle$$

It is clear that the basis $\left\{\left|w^{\mathbf{R}_m}\right\rangle\right\}$ and $\left\{\left|\tilde{w}^{\mathbf{R}_m}\right\rangle\right\}$ can be different.

The basis above is ordered in band index and fixed in $\mathbf{R_m}$ ($\mathbf{k}$ in bloch wave) index.

"Problem" of Wannier Functions

Noting

Although, $\left\{\left|w^{\mathbf{R}_m}\right\rangle\right\}$ and $\left\{\left|\tilde{w}^{\mathbf{R}_m}\right\rangle\right\}$ are two different basis, they actually describe the same subspace. Since the orthogonality of Wannier function do not depend on the arbitrary phase $\phi_i(\mathbf{k})$, those two different basis are, in fact, related via a unitary matrix.

$$\begin{pmatrix} \left|\tilde{w}_1^{\mathbf{R}_m}\right\rangle \\ \left|\tilde{w}_2^{\mathbf{R}_m}\right\rangle \\ \vdots \\ \left|\tilde{w}_{N_{bands}}^{\mathbf{R}_m}\right\rangle \end{pmatrix} = \widehat{\mathbf{U}}^{\mathbf{R}_m} \begin{pmatrix} \left|w_1^{\mathbf{R}_m}\right\rangle \\ \left|w_2^{\mathbf{R}_m}\right\rangle \\ \vdots \\ \left|w_{N_{bands}}^{\mathbf{R}_m}\right\rangle \end{pmatrix} \tag{13}$$

Where $\widehat{\mathbf{U}}^{\mathbf{R}_m}$ is a unitary matrix.

"Maximally Localized" Wannier Function

"Maximally Localized" Wannier Function (MLWF) is one simple solution for constructing Wannier functions from its arbitrary phase problem.

Why Localized Basis?

- Decrease the calculation complexity.
- Many physical processes are only related to local properties.

Easy to Localized?

The process that localized the wannier functions is actually not that easy as you may think. Later, we will introduce you the maximally localized method that adapted by *Wannier90*[a], a well-known wannier functions fitting package.

[a] *An updated version of Wannier90: A tool for obtaining maximally-localized Wannier functions, AA Mostofi, JR Yates, G Pizzi, YS Lee, I Souza, D Vanderbilt, N Marzari, Comput. Phys. Commun. 185, 2309 (2014)*

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Degree of "Localization"

The "Localized" here means the wave function decay very quickly. Thus, one can use the variance to describe the degree of such a "Localization".

$$\Omega = \sum_{i=1}^{N_{bands}} \langle \widehat{\mathbf{r}}^2 \rangle_i - \langle \widehat{\mathbf{r}} \rangle_i^2 \tag{14}$$

Where $\langle \widehat{\mathcal{O}} \rangle_i = \left\langle w_i^{\mathbf{0}} \middle| \widehat{\mathcal{O}} \middle| w_i^{\mathbf{0}} \right\rangle$

Methods

Minimized Ω, one can get the well behaved MLWF.

Split the variance Ω

Let,

$$\Omega = \Omega_I + \widetilde{\Omega}$$

$$\Omega_I = \sum_{i=1}^{N_{bands}} \left[\langle \mathbf{r}^2 \rangle_i - \sum_{j,\mathbf{R}} \left| \langle w_j^{\mathbf{R}} | \widehat{\mathbf{r}} | w_i^{\mathbf{0}} \rangle \right|^2 \right] \tag{15}$$

$$\widetilde{\Omega} = \sum_{i=1}^{N_{bands}} \sum_{j \neq i, \mathbf{R} \neq \mathbf{0}} \left| \langle w_j^{\mathbf{R}} | \widehat{\mathbf{r}} | w_i^{\mathbf{0}} \rangle \right|^2$$

Noting

Clearly, the second term $\widetilde{\Omega}$ is always positive. The clever part of this division is that, Ω_I is both invariant and always positive.

Question

Why Ω_I is both invariant and always positive?

Special Properties of $\Omega_{\mathbf{I}}$

Question

Why Ω_I is both invariant and always positive?

Answer

To answer this question, firstly, we need to build up two projection operators, $\widehat{P}$ and $\widehat{Q}$.

$$\widehat{P} = \sum_{i=1}^{N_{bands}} \sum_{\mathbf{R}} \left|w_i^{\mathbf{R}}\right\rangle \left\langle w_i^{\mathbf{R}}\right| = \sum_{i=1}^{N_{bands}} \sum_{\mathbf{k}} \left|\psi_i^{\mathbf{k}}\right\rangle \left\langle \psi_i^{\mathbf{k}}\right| \tag{16a}$$

$$\widehat{Q} = 1 - \widehat{P} \tag{16b}$$

Use projection operators, the Ω_I can be rewritten as:

$$\Omega_I = \sum_{i=1}^{N_{bands}} \sum_{\alpha=1}^{3} \left\langle w_i^{\mathbf{0}} \middle| \widehat{\mathbf{r}}_\alpha \widehat{Q}\, \widehat{\mathbf{r}}_\alpha \middle| w_i^{\mathbf{0}} \right\rangle \tag{17}$$

Special Properties of $\Omega_{\mathbf{I}}$

Answer

- Positive

$$\begin{aligned}\Omega_I &= \sum_{i=1}^{N_{bands}} \sum_{\alpha=1}^{3} \left\langle w_i^{\mathbf{0}} \middle| \hat{\mathbf{r}}_\alpha \hat{Q} \hat{\mathbf{r}}_\alpha \middle| w_i^{\mathbf{0}} \right\rangle \\ &= \sum_{i=1}^{N_{bands}} \sum_{\alpha=1}^{3} \left\langle w_i^{\mathbf{0}} \middle| \hat{\mathbf{r}}_\alpha \hat{Q} \hat{Q} \hat{\mathbf{r}}_\alpha \middle| w_i^{\mathbf{0}} \right\rangle \\ &= \sum_{i=1}^{N_{bands}} \sum_{\alpha=1}^{3} \left\| \left| \hat{Q} \hat{\mathbf{r}}_\alpha \middle| w_i^{\mathbf{0}} \right\rangle \right\|^2 > 0\end{aligned}$$

- Invariant
  The next question is why the Ω_I is invariant about the "gauge transformation".

Special Properties of Ω_I

Answer

$$\Omega_I = \sum_{i=1}^{N_{bands}} \sum_{\alpha=1}^{3} \left\langle w_i^{\mathbf{0}} \middle| \hat{\mathbf{r}}_\alpha \hat{Q}\, \hat{\mathbf{r}}_\alpha \middle| w_i^{\mathbf{0}} \right\rangle$$

$$= \sum_{i=1}^{N_{bands}} \sum_{\alpha=1}^{3} \left\langle w_i^{\mathbf{0}} \middle| \hat{P}\, \hat{\mathbf{r}}_\alpha \hat{Q}\, \hat{\mathbf{r}}_\alpha \middle| w_i^{\mathbf{0}} \right\rangle$$

$$= \sum_{\alpha=1}^{3} \mathrm{Tr}_c \left[\hat{P}\, \hat{\mathbf{r}}_\alpha \hat{Q}\, \hat{\mathbf{r}}_\alpha \right]$$

The c of Tr_c here indicated that only calculate the trace inside one unit cell. Remember that, the gauge transformation is actually a unitary one. Under that, the trace of any operator (or their product) is invariant.

A New Question

But still, there is another question: when will the Ω_I change?

Parctical expression in k-space

Now Let's try to express the Ω using $\left|u_i^{\mathbf{k}}\right\rangle$ (in k space).
Before that, we need some math preparation.

Math Prepare

Let $\mathbf{b}$ be a vector connecting a k-point to one of its near neighbours, and by an appropriate choice of a weight w_b associated with each shell $b = |\mathbf{b}|$, it satisfied,

$$\sum_{\mathbf{b}} w_b \mathbf{b}_\alpha \mathbf{b}_\beta = \delta_{\alpha\beta} \tag{18}$$

Then the gradiant of $f(\mathbf{k})$ can be expressed as:[a]

$$\nabla f(\mathbf{k}) = \sum_{\mathbf{b}} w_b \mathbf{b} \left[f(\mathbf{b}+\mathbf{k}) - f(\mathbf{b}) \right] \tag{19}$$

[a] *Maximally-localized generalized Wannier functions for composite energy bands, N Marzari, D Vanderbilt,* `https://arxiv.org/abs/cond-mat/9707145`

Parctical expression in k-space

$$\nabla f(\mathbf{k}) = \sum_{\mathbf{b}} w_b \mathbf{b} \left[f(\mathbf{b}+\mathbf{k}) - f(\mathbf{b}) \right]$$

Remember,

$$\begin{aligned} \left\langle w_i^{\mathbf{k}} \middle| \widehat{\mathbf{r}} \middle| w_j^{\mathbf{0}} \right\rangle &= \mathrm{i} \frac{V}{(2\pi)^2} \int_{BZ} d^3k \, \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{R}} \left\langle u_i^{\mathbf{k}} \middle| \nabla_{\mathbf{k}} \middle| u_j^{\mathbf{k}} \right\rangle \\ &= \frac{\mathrm{i}}{N_{\mathbf{k}}} \sum_{\mathbf{k}} \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{R}} \left\langle u_i^{\mathbf{k}} \middle| \nabla_{\mathbf{k}} \middle| u_j^{\mathbf{k}} \right\rangle \end{aligned}$$

which means,

$$\begin{aligned} \langle \widehat{\mathbf{r}} \rangle_i &= \frac{\mathrm{i}}{N_{\mathbf{k}}} \sum_{\mathbf{k}} \left\langle u_i^{\mathbf{k}} \middle| \nabla_{\mathbf{k}} \middle| u_i^{\mathbf{k}} \right\rangle \\ &= \frac{\mathrm{i}}{N_{\mathbf{k}}} \sum_{\mathbf{k},\mathbf{b}} w_b \mathbf{b} \left[\left\langle u_i^{\mathbf{k}} \middle| u_i^{\mathbf{k}+\mathbf{b}} \right\rangle - 1 \right] \end{aligned} \tag{20}$$

Parctical expression in k-space

$$\langle \widehat{\mathbf{r}} \rangle_i = \frac{\mathrm{i}}{N_{\mathbf{k}}} \sum_{\mathbf{k},\mathbf{b}} w_b \mathbf{b} \left[\left\langle u_i^{\mathbf{k}} \middle| u_i^{\mathbf{k}+\mathbf{b}} \right\rangle - 1 \right]$$

Use the same technique, we can get,

$$|\nabla_{\mathbf{k}} f(\mathbf{k})|^2 = \sum_{\mathbf{b}} w_b \left[f(\mathbf{k}+\mathbf{b}) - f(\mathbf{k}) \right]^2 \tag{21}$$

$$\begin{aligned} \langle \widehat{\mathbf{r}^2} \rangle_i &= -\frac{V}{(2\pi)^3} \int_{BZ} d^3k \ \left\langle u_i^{\mathbf{k}} \middle| \nabla_{\mathbf{k}}^2 \middle| u_i^{\mathbf{k}} \right\rangle \\ &= \frac{V}{(2\pi)^3} \int_{BZ} d^3k \left\| \nabla_{\mathbf{k}} \left| u_i^{\mathbf{k}} \right\rangle \right\|^2 \\ &= \frac{1}{N_{\mathbf{k}}} \sum_{\mathbf{k},\mathbf{b}} w_b \left\{ 2 - Re \left[\left\langle u_i^{\mathbf{k}} \middle| u_i^{\mathbf{k}+\mathbf{b}} \right\rangle \right] \right\} \end{aligned} \tag{22}$$

Expression Approximation in k-space

$$\langle \hat{\mathbf{r}} \rangle_j = \frac{\mathrm{i}}{N_{\mathbf{k}}} \sum_{\mathbf{k},\mathbf{b}} w_b \mathbf{b} \left[\langle u_j^{\mathbf{k}} | u_j^{\mathbf{k}+\mathbf{b}} \rangle - 1 \right]$$

If we define $\langle u_i^{\mathbf{k}} | u_j^{\mathbf{k}+\mathbf{b}} \rangle = M_{ij}(\mathbf{k}, \mathbf{b})$, the expression (20) can be rewritten as:

$$\langle \hat{\mathbf{r}} \rangle_j = -\frac{1}{N_{\mathbf{k}}} \sum_{\mathbf{k},\mathbf{b}} w_b \mathbf{b} \, \mathrm{Im}[ln M_{jj}(\mathbf{k}, \mathbf{b})] \tag{23}$$

Explanation

Use Taylor expansion,

$$ln(1 + \mathrm{i}x) = \mathrm{i}x - \frac{1}{2}x^2 + \mathrm{i}\mathcal{O}(x^3) + \mathcal{O}(x^4)$$

for small x, $\mathrm{Im}[ln(1 + \mathrm{i}x)] \approx x$.

$-\mathrm{i}\left(\langle u_i^{\mathbf{k}} | u_i^{\mathbf{k}+\mathbf{b}} \rangle - 1\right) \approx -\mathrm{i} \langle u_i^{\mathbf{k}} | \nabla_{\mathbf{k}} | u_i^{\mathbf{k}} \rangle \cdot \mathbf{b}$ is a small number.

Expression Approximation in k-space

$$\langle \hat{\mathbf{r}} \rangle_j = -\frac{1}{N_{\mathbf{k}}} \sum_{\mathbf{k},\mathbf{b}} w_b \mathbf{b}\, \mathrm{Im}[lnM_{jj}(\mathbf{k},\mathbf{b})]$$

Noting

The $\langle \hat{\mathbf{r}} \rangle_j$ here is called wannier center for j^{th} Wannier functions.

Similarly,

$$\langle \hat{\mathbf{r}}^2 \rangle_j = \frac{1}{N_{\mathbf{k}}} \sum_{\mathbf{k},\mathbf{b}} w_b \left\{ 1 - |M_{jj}(\mathbf{k},\mathbf{b})|^2 + (\mathrm{Im}[lnM_{jj}(\mathbf{k},\mathbf{b})])^2 \right\} \tag{24a}$$

$$\Omega_I = \frac{1}{N_{\mathbf{k}}} \sum_{\mathbf{k},\mathbf{b}} w_b \left[N_{bands} - \sum_{i,j=1}^{N_{bands}} |M_{ij}(\mathbf{k},\mathbf{b})|^2 \right] \tag{24b}$$

$$\widetilde{\Omega} = \frac{1}{N_{\mathbf{k}}} \sum_{\mathbf{k},\mathbf{b}} w_b \left[\sum_{i=1}^{N_{bands}} \left(- \mathrm{Im}[lnM_{ii}(\mathbf{k},\mathbf{b})] - \mathbf{b} \cdot \langle \mathbf{r} \rangle_i \right)^2 + \sum_{i \neq j}^{N_{bands}} |M_{ij}(\mathbf{k},\mathbf{b})|^2 \right] \tag{24c}$$

Key Expression for Understanding $\Omega_{\mathbf{I}}$

$$\Omega_I = \frac{1}{N_{\mathbf{k}}} \sum_{\mathbf{k},\mathbf{b}} w_b \left[N_{bands} - \sum_{i,j=1}^{N_{bands}} |M_{ij}(\mathbf{k},\mathbf{b})|^2 \right]$$

Noting

If we define $\widehat{P}_{\mathbf{k}} = \sum_{i=1}^{N_{bands}} \left|u_i^{\mathbf{k}}\right\rangle \left\langle u_i^{\mathbf{k}}\right|$, $\widehat{Q}_{\mathbf{k}} = 1 - \widehat{P}_{\mathbf{k}}$, then,

$$\Omega_I = \frac{1}{N_{\mathbf{k}}} \sum_{\mathbf{k},\mathbf{b}} w_b \mathrm{Tr}\left[\widehat{P}_{\mathbf{k}} \widehat{Q}_{\mathbf{k}+\mathbf{b}}\right] \tag{25}$$

The expression (25) plays a critical role in understanding the physical meaning of Ω_I.

Outer Energy Window

The above description is sufficient to obtain MLWF for an isolated set of bands, which means, the index "i" of $\left|u_i^{\mathbf{k}}\right\rangle$ and $\left|w_i^{\mathbf{R}}\right\rangle$ are both represent the band order. But in some of the case, such as in the metallic system, one can hardly divide the bands individually. ("The Case of Entangled Bands")
In that case, the "disentanglement" technique needs to be applied.

Methods

- An energy window (the "outer window") is defined by the user such that at each k-point there are $N_{win}^{(\mathbf{k})} (\geqslant N)$ states within the window.
- An orthonormal set of N Bloch states is obtained at each k-point, defining an N-dimensional subspace $S_{\mathbf{k}}$.

$$\left|u_i^{\mathbf{k}}\right\rangle = \sum_{j \in N_{win}^{(\mathbf{k})}} \mathbf{U}_{ji}^{dis(\mathbf{k})} \left|u_j^{(origin)\mathbf{k}}\right\rangle \tag{26}$$

Where $\mathbf{U}^{dis(\mathbf{k})}$ is a rectangular $N_{win}^{(\mathbf{k})} \times N$ matrix.

$\Omega_{\mathbf{I}}$ as a Function of $S_{\mathbf{k}}$

Question we asked before

Under what condition, will the Ω_I change?

Answer

$$\Omega_I = \frac{1}{N_{\mathbf{k}}} \sum_{\mathbf{k},\mathbf{b}} w_b \mathrm{Tr}\left[\widehat{P}_{\mathbf{k}} \widehat{Q}_{\mathbf{k}+\mathbf{b}}\right]$$

The answer is quite straightforward. Since the Ω_I is a trace about the subspace. Only change the basis via a unitary transformation will not change such trace. But if we change the subspace itself, then, all most certainly, Ω_I will be changed. This analysis also inspire that, we can actually regard the Ω_I as a function of subspace $S_{\mathbf{k}}$.

$$\Omega_I = \Omega_I(S_{\mathbf{k}})$$

Under a given original bloch wave data set, which means a fixed $\left|u_j^{(origin)\mathbf{k}}\right\rangle$, by optimizing the $\mathbf{U}^{dis(\mathbf{k})}$, Ω_I can then be minimized, theoritically.

Physical Meaning of Minimising $\Omega_{\mathbf{I}}$

A Simple Description

$$\Omega_I = \frac{1}{N_{\mathbf{k}}} \sum_{\mathbf{k},\mathbf{b}} w_b \mathrm{Tr}\left[\hat{P}_{\mathbf{k}} \hat{Q}_{\mathbf{k+b}}\right]$$

It can be seen very clearly that, Ω_I is a measure of the degree of mismatch between the subspace $S_{\mathbf{k}}$ and $S_{\mathbf{k+b}}$. Minimising Ω_I corresponds to choosing self-consistently at every $\mathbf{k}$ the subspace that has maximum overlap as $\mathbf{k}$ is varied. That is, Ω_I is small insofar as $S_{\mathbf{k}}$ is nearly independent of k.

Not Clear Enough

The explanation above is still not deep enough, for the clear understanding of it is really a long story, and needs lots of mathematics background. But it is still worth noting that, the optimizing of Ω_I is actually related to the smooth of Barry Phase.[a]

[a] *Maximally-localized generalized Wannier functions for composite energy bands, N Marzari, D Vanderbilt, https://arxiv.org/abs/cond-mat/9707145*

Inner Energy Window

Noting

It may be the case that the energy bands of the projected subspace do not correspond to any of the original energy bands due to mixing between states. In order to preserve exactly the properties of a system within a given energy range (e.g., around the Fermi level), an "inner energy window" is introduced. States lying within this inner, or frozen, energy window are included unchanged in the projected subspace.[a]

[a] *Maximally localized Wannier functions for entangled energy bands, S Ivo, M Nicola, and V David, Phys. Rev. B, 65, 035109*

After minimized the Ω_I under the inner and outer window, which also means selecting the best subspace set for the system, we can now start to minimize the $\widetilde{\Omega}$ by a unitary matrix $\mathbf{U^k}$ inside each subspace.

Methods Conclusion

- By minimizing Ω, the Wannier function can be localized tightly.
- During the minimization, *Wannier90* will first try to use $\mathbf{U}^{dis(\mathbf{k})}$ generate the best subspace set for the system, which is corresponding to minimize Ω_I.
- The format of $\mathbf{U}^{dis(\mathbf{k})}$ is decided by the "Outer & Inner Window".
- Once the best subspace set is selected, a unitary matrix $\mathbf{U}^{\mathbf{k}}$ inside each subspace will be used to minimize the $\widetilde{\Omega}$.
- After this two process, we can regrad the Ω as a minimized one.
- All of the minimize process is operated in k space, for it is easier and less complex than that in real space.

Hamiltonian For MLWF

$$\widehat{H}^{(W)}(\mathbf{k}) = \mathbf{U}^{(\mathbf{k})\dagger}\mathbf{U}^{\mathbf{dis}(\mathbf{k})\dagger}\widehat{H}(\mathbf{k})\mathbf{U}^{\mathbf{dis}(\mathbf{k})}\mathbf{U}^{(\mathbf{k})} \tag{27}$$

More Technique Questions

Question1

Is there any other way to minimize Ω? (instand of split it into Ω_I & $\widetilde{\Omega}$)

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How to obtain the best $\mathbf{U}^{\mathbf{dis}(\mathbf{k})}$ and $\mathbf{U}^{(\mathbf{k})}$?

Answer1

Yes, of course! Actually, you can directly minimize Ω overall.[a]

[a] *Partly Occupied Wannier Functions, K S Thygesen, L B Hansen, and K W Jacobsen, Phys. Rev. Lett., 94, 026405*

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Answer2

That is another long story.[a]

[a] *Maximally localized Wannier functions for entangled energy bands, S Ivo, M Nicola, and V David, Phys. Rev. B, 65, 035109*

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Calculation Strategy

Process for Wannier Calculation

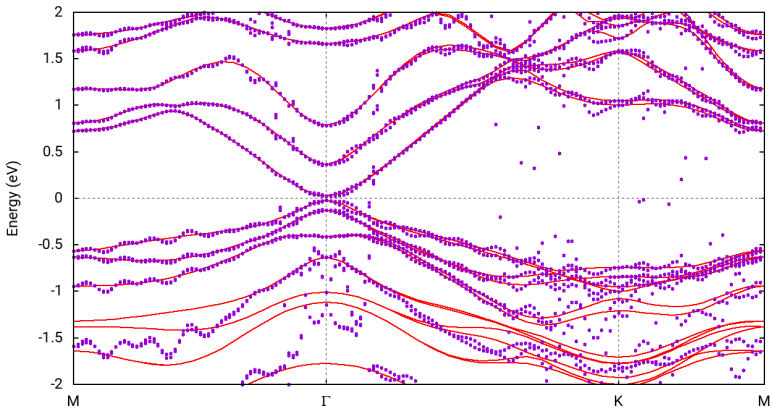
- Calculate Bloch Wave use DFT. (VASP[a], ABINIT, QE,...)
- Project Bloch Wave to Wannier Functions. (*Wannier90*[b])
- Post Process. (WannierTools[c], OWL, TideBird)

[a] `https://www.vasp.at`
[b] `http://www.wannier.org`
[c] `https://github.com/quanshengwu/wannier_tools`

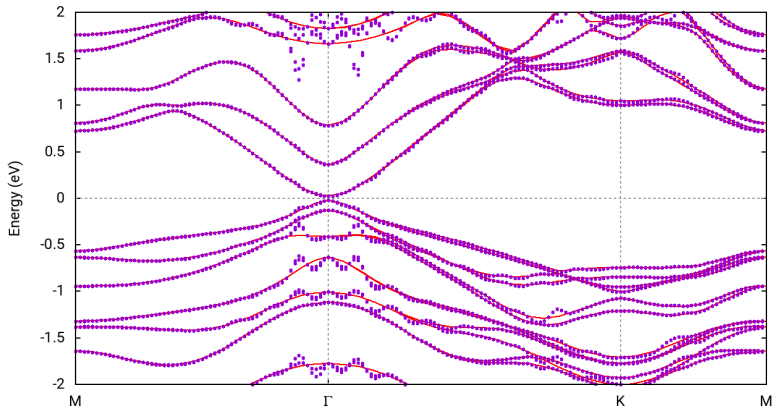
A Script for WF Fitting

`https://github.com/kYangLi/AbInitioCalcScript/tree/master/`
`\emph{Wannier90}`

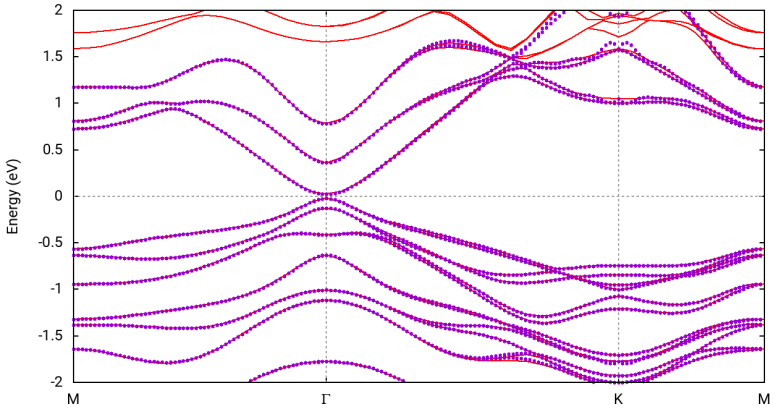
Fitting Result



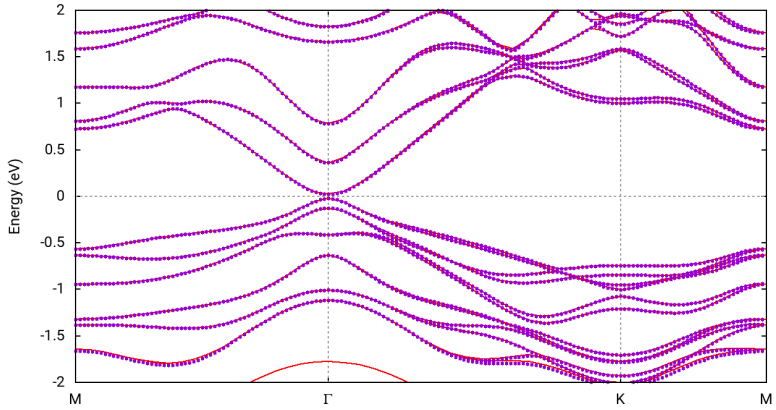
(a) froz_win:$[-1.0, 3.0]$



(b) froz_win:$[-2.0, 2.0]$



(c) froz_win:$[-1.5, 1.5]$



(d) froz_win:$[-1.5, 2.0]$

Figure: Bands Calc. by VASP and *Wannier90*

A Useful Adv. for WF Fitting

As The Cow Says:

```
 ---------------------------------------
/ Next time you start a wannier fitting \
| project, remember to name the project |
\ folder as ``Lucky''.                  /
 ---------------------------------------
        \   ^__^
         \  (oo)\_______
            (__)\       )\/\
                ||----w |
                ||     ||
```

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Summary

Summary

- Wannier functions are Fourier transforms of the Bloch eigenstate.
- Wannier functions are not uniquely defined.
- "Maximally Localized" Wannier Function (MLWF) is one simple solution for constructing a well-performed Wannier functions.
- The process of obtaining MLWF can be divided into two steps: optimize subspace, after which, optimize inside each fixed subspace.
- *Wannier90* is a widely used Wannier fitting package.
- Wannier fitting needs a lot of experiment and, sometimes, is kind of tricky.

Open Source Declaration

Declaration

This slides is completely open-source and protected by GPL3.0. You can share or modify it based on any non-commercial purpose.

The source code and references are available on related GitHub repository:
https://github.com/kYangLi/PublicPresentation/tree/master/WannierFunctions