wannier-second quantization

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In this article we show the equivalence of wannier function and second quantization when constructing a tight-binding model. The "equivalence" means that their Hamiltonians differ by a basis transformation:

$$H_w = QH_sQ^\dagger, \quad Q^\dagger Q = id. \tag{1}$$

First the two Hamiltonians are

$$H_w = \sum_{ij} w_{ij} \left|i_w\right\rangle \left\langle j_w\right|; \tag{2}$$

$$H_s = \sum_{ij} h_{ij} \left|i_s\right\rangle \left\langle j_s\right|. \tag{3}$$

We only need to show that

$$w_{mn} = \sum_{ij} \left\langle m_w|i_s\right\rangle h_{ij} \left\langle j_s|n_w\right\rangle \Leftrightarrow [w]_{mn} = ([Q][h][Q^\dagger])_{mn}, \tag{4}$$

here

$$Q_{ij} = \left\langle i_w|j_s\right\rangle. \tag{5}$$

In wannier functions we have

$$w_{ij} = \sum_{\mathbf{R}} H_{ij}(\mathbf{R})\mathrm{e}^{i\mathbf{k}\cdot\mathbf{R}}, \tag{6}$$

where

$$\mathbf{R} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3 \tag{7}$$

and

$$H_{ij}(\mathbf{R}) = \langle \mathbf{0}|H|\mathbf{R}\rangle u_i(\mathbf{0})^* u_j(\mathbf{0}). \tag{8}$$

In second quantization we have

$$h_{ij} = \sum_{\mathbf{R}_j} t_{ij}(\mathbf{R}_i, \mathbf{R}_j)\mathrm{e}^{i\mathbf{k}\cdot(\mathbf{R}_j - \mathbf{R}_i)}. \tag{9}$$

If their are only one site(or atom) in each unit cell, we would have $\mathbf{R}_i = \mathbf{0}$ and $\mathbf{R}_j = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3$. Then

$$h_{ij} = \sum_{\mathbf{R}} t(\mathbf{R})\mathrm{e}^{i\mathbf{k}\cdot\mathbf{R}}. \tag{10}$$

We must have $t_{ij}(\mathbf{R}) = H_{ij}(\mathbf{R})$ to acquire the equivalence and $Q = id$.

The problem arises when one has multiple sites(atoms) in each unit cell. WLOG we only have one orbital on each site, so that we can label that orbital by its atom. Now, each wannier orbital is written as $|p, \mathbf{R}_q\rangle$ here p is the label of the atom and $\mathbf{R}_q$ is the position of that unit cell. Each second quantization orbital is written as $|r, \mathbf{R}_s\rangle$ where r is the lablel of the atom and $\mathbf{R}_s$ is the position of the atom. We always have $\mathbf{R}_s = \mathbf{R}_q + \mathbf{r}_r$.

Now

$$h_{ij} = \sum_{\mathbf{R}} t_{ij}(\mathbf{r}_i, \mathbf{r}_j + \mathbf{R})\mathrm{e}^{i\mathbf{k}\cdot\mathbf{R}}\mathrm{e}^{i\mathbf{k}\cdot(\mathbf{r}_j - \mathbf{r}_i)}. \tag{11}$$

Impose $t_{ij}(\mathbf{r}_i, \mathbf{r}_j + \mathbf{R}) = H_{ij}(\mathbf{R})$ and then

$$h_{ij} = \sum_{\mathbf{R}} H_{ij}(\mathbf{R}) \mathrm{e}^{i\mathbf{k}\cdot\mathbf{R}} \mathrm{e}^{i\mathbf{k}\cdot(\mathbf{r}_j - \mathbf{r}_i)} = w_{ij} \mathrm{e}^{i\mathbf{k}\cdot(\mathbf{r}_j - \mathbf{r}_i)}. \tag{12}$$

Now the transformation is clear, but it remains to be shown that $[h]$ and $[w]$ differ by a similar transformation. Very obviously

$$h_{mn} = \sum_{ij} w_{ij} \delta_{mi} \mathrm{e}^{-i\mathbf{k}\cdot\mathbf{r}_m} \delta_{nj} \mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}_n}. \tag{13}$$

Defining

$$Q_{ij} = \delta_{ij} \mathrm{e}^{-i\mathbf{k}\cdot\mathbf{r}_i}, \quad Q^{\dagger}_{ij} = \delta_{ji} \mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}_j} \tag{14}$$

then

$$h_{mn} = \sum_{ij} w_{ij} Q_{mi} Q^{\dagger}_{jn}. \tag{15}$$

It is obvious that $Q^{\dagger} Q = id$.

Take the example: 1-D string with site A at 0 and B at 1 in the unit cell. $d(A, B) = 1$ and $\mathbf{a}_1 = 1$. Using wannier function we have

$$H_w = \begin{bmatrix} 0 & 1 + \mathrm{e}^{-2ik} \\ 1 + e^{2ik} & E \end{bmatrix}. \tag{16}$$

Using second quantization we have

$$H_s = \begin{bmatrix} 0 & 2\cos(k) \\ 2\cos(k) & E \end{bmatrix}. \tag{17}$$

So

$$Q = \begin{bmatrix} 1 & 0 \\ 0 & \mathrm{e}^{-ik} \end{bmatrix}, \tag{18}$$

and

$$QH_wQ^{\dagger} = \begin{bmatrix} 1 & 0 \\ 0 & \mathrm{e}^{-ik} \end{bmatrix} \begin{bmatrix} 0 & 1 + \mathrm{e}^{-2ik} \\ 1 + e^{2ik} & E \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & \mathrm{e}^{ik} \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & \mathrm{e}^{-ik} \end{bmatrix} \begin{bmatrix} 0 & 2\cos k \\ 1 + e^{2ik} & E\mathrm{e}^{ik} \end{bmatrix} = H_s. \tag{19}$$