WannierExcitonModel.jl - Theory

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Contents

1 Introduction

This is the Physical background for WannierExcitonModel.jl.

2 Tight Binding Model

We assume that reader have the basic knowledge of "Band Theory" and "Tight-Binding Model", So this chaper is mainly used to define the relevant notations.

2.1 Poison summation

Finite case:

$$\begin{aligned} \sum_{\boldsymbol{R}} e^{i(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{R}} &= N\delta_{\boldsymbol{k}\boldsymbol{k}'} \\ \sum_{\boldsymbol{k}} e^{i\boldsymbol{k}\cdot(\boldsymbol{R}-\boldsymbol{R}')} &= N\delta_{\boldsymbol{R}\boldsymbol{R}'} \end{aligned} \tag{1}$$

Infinite case:

$$\begin{aligned} \sum_{\boldsymbol{R}} e^{i(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{R}} &= \frac{(2\pi)^3}{V}\delta(\boldsymbol{k}-\boldsymbol{k}') \\ \frac{V}{(2\pi)^3}\int \mathrm{d}\boldsymbol{k} e^{i\boldsymbol{k}\cdot(\boldsymbol{R}-\boldsymbol{R}')} &= \delta_{\boldsymbol{R}\boldsymbol{R}'} \end{aligned} \tag{2}$$

2.2 Band state

For the case where the system is infinite, we define

$$\begin{aligned} \text{Orthonormality: } \langle m\boldsymbol{k}|n\boldsymbol{k}'\rangle &= \frac{(2\pi)^3}{V}\delta_{mn}\delta(\boldsymbol{k}-\boldsymbol{k}') \\ \text{Completeness: } \hat{\mathcal{I}} &= \frac{V}{(2\pi)^3}\int \mathrm{d}\boldsymbol{k} \sum_n |n\boldsymbol{k}\rangle\langle n\boldsymbol{k}| \end{aligned} \tag{3}$$

where $|n\boldsymbol{k}\rangle$ is the single partical Bloch state. Under unitary transformation $U_{in}^{\boldsymbol{k}}$, these two equations maintain the formation:

$$\begin{aligned} |n\boldsymbol{k}\rangle = \sum_i U_{in}^{\boldsymbol{k}} |i\boldsymbol{k}\rangle &,\ |i\boldsymbol{k}\rangle = \sum_n U_{in}^{\boldsymbol{k}*} |n\boldsymbol{k}\rangle \\ \text{Orthonormality: } \langle i\boldsymbol{k}|j\boldsymbol{k}'\rangle &= \frac{(2\pi)^3}{V}\delta_{ij}\delta(\boldsymbol{k}-\boldsymbol{k}') \\ \text{Completeness: } \hat{\mathcal{I}} &= \frac{V}{(2\pi)^3}\int \mathrm{d}\boldsymbol{k} \sum_i |i\boldsymbol{k}\rangle\langle i\boldsymbol{k}| \end{aligned} \tag{4}$$

We can define wannier states from Bloch states, and deduce its orthonormality and completeness:

$$\begin{aligned} |i\boldsymbol{k}\rangle = \sum_{\boldsymbol{R}} e^{i\boldsymbol{k}\cdot\boldsymbol{R}}|i\boldsymbol{R}\rangle &,\ |i\boldsymbol{R}\rangle = \frac{V}{(2\pi)^3}\int \mathrm{d}\boldsymbol{k} e^{-i\boldsymbol{k}\cdot\boldsymbol{R}}|i\boldsymbol{k}\rangle \\ \text{Orthonormality: } \langle i\boldsymbol{R}|j\boldsymbol{R}'\rangle &= \delta_{ij}\delta_{\boldsymbol{R}\boldsymbol{R}'} \\ \text{Completeness: } \hat{\mathcal{I}} &= \sum_{i\boldsymbol{R}} |i\boldsymbol{R}\rangle\langle i\boldsymbol{R}| \end{aligned} \tag{5}$$

2.2.1 Bloch state $|n\boldsymbol{k}\rangle$

We can get the numerical vector form of Bloch function $|n\boldsymbol{k}\rangle$ with wannier basis.

$$|n\boldsymbol{k}\rangle = \sum_i U_{in}^{\boldsymbol{k}}|i\boldsymbol{k}\rangle = \sum_{i\boldsymbol{R}} U_{in}^{\boldsymbol{k}} e^{i\boldsymbol{k}\cdot\boldsymbol{R}}|i\boldsymbol{R}\rangle \tag{6}$$

With $\hat{H}|n\boldsymbol{k}\rangle = E_{n\boldsymbol{k}}|n\boldsymbol{k}\rangle$, we can get

$$
\begin{aligned}
\langle i\boldsymbol{k}'|\, H\, |n\boldsymbol{k}\rangle &= \sum_j U_{jn}^{\boldsymbol{k}} \sum_{\boldsymbol{R}'\boldsymbol{R}} e^{i(\boldsymbol{k}\cdot\boldsymbol{R}-\boldsymbol{k}'\cdot\boldsymbol{R}')} \langle i\boldsymbol{R}'|\, H\, |j\boldsymbol{R}\rangle \\
&= \sum_j U_{jn}^{\boldsymbol{k}} \sum_{\boldsymbol{R}'\boldsymbol{R}} e^{i(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{R}'} e^{i\boldsymbol{k}\cdot(\boldsymbol{R}-\boldsymbol{R}')} \langle i\boldsymbol{0}|\, H\, |j\boldsymbol{R}-\boldsymbol{R}'\rangle \\
&= \sum_j U_{jn}^{\boldsymbol{k}} \sum_{\boldsymbol{R}_0} e^{i(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{R}_0} \sum_{\boldsymbol{R}} e^{i\boldsymbol{k}\cdot\boldsymbol{R}} \langle i\boldsymbol{0}|\, H\, |j\boldsymbol{R}\rangle \\
&= \frac{(2\pi)^3}{V}\delta(\boldsymbol{k}-\boldsymbol{k}') \sum_j H_{ij}^{\boldsymbol{k}} U_{jn}^{\boldsymbol{k}} \\
\langle i\boldsymbol{k}'|\, E_{n\boldsymbol{k}}\, |n\boldsymbol{k}\rangle &= \frac{(2\pi)^3}{V}\delta(\boldsymbol{k}-\boldsymbol{k}') E_{n\boldsymbol{k}} U_{in}^{\boldsymbol{k}} \\
&\Rightarrow \sum_j H_{ij}^{\boldsymbol{k}} U_{jn}^{\boldsymbol{k}} = E_{n\boldsymbol{k}} U_{in}^{\boldsymbol{k}}
\end{aligned} \tag{7}
$$

where

$$
H_{ij}^{\boldsymbol{k}} = \sum_{\boldsymbol{R}} e^{i\boldsymbol{k}\cdot\boldsymbol{R}} \langle i\boldsymbol{0}|\, H\, |j\boldsymbol{R}\rangle \tag{8}
$$

2.2.2 $|u_{n\boldsymbol{k}}\rangle = e^{-i\boldsymbol{k}\cdot\hat{\boldsymbol{r}}} |n\boldsymbol{k}\rangle$

Now we try to get $|u_{n\boldsymbol{k}}\rangle$, the periodic part of Bloch function $|n\boldsymbol{k}\rangle$.

$$
\begin{aligned}
|u_{n\boldsymbol{k}}\rangle = e^{-i\boldsymbol{k}\cdot\hat{\boldsymbol{r}}} |n\boldsymbol{k}\rangle &= \sum_i U_{in}^{\boldsymbol{k}} e^{-i\boldsymbol{k}\cdot\hat{\boldsymbol{r}}} |i\boldsymbol{k}\rangle = \sum_i U_{in}^{\boldsymbol{k}} |u_{i\boldsymbol{k}}\rangle \\
|u_{i\boldsymbol{k}}\rangle &= \sum_{\boldsymbol{R}} e^{i\boldsymbol{k}\cdot(\boldsymbol{R}-\hat{\boldsymbol{r}})} |i\boldsymbol{R}\rangle
\end{aligned} \tag{9}
$$

Whether in the field of physical theories or mathematical theories, we only need the unitcell's inner product of $|u_{n\boldsymbol{k}}\rangle$ between the adjacent $\boldsymbol{k}$, which can be used to calculate physical quantities such as the Berry connection. So we have

$$
\begin{aligned}
\lim_{\boldsymbol{k}\to\boldsymbol{k}'} \langle u_{i\boldsymbol{k}'}|u_{j\boldsymbol{k}}\rangle_{uc} &= \frac{1}{\sum_{\boldsymbol{R}}} \langle u_{i\boldsymbol{k}'}|u_{j\boldsymbol{k}}\rangle \\
&= \frac{1}{\sum_{\boldsymbol{R}}} \sum_{\boldsymbol{R}'\boldsymbol{R}} e^{i(\boldsymbol{k}\cdot\boldsymbol{R}-\boldsymbol{k}'\cdot\boldsymbol{R}')} \langle i\boldsymbol{R}'|\, e^{i(\boldsymbol{k}'-\boldsymbol{k})\cdot\hat{\boldsymbol{r}}}\, |j\boldsymbol{R}\rangle \\
&= \frac{1}{\sum_{\boldsymbol{R}}} \sum_{\boldsymbol{R}_0\boldsymbol{R}} e^{i\boldsymbol{k}\cdot\boldsymbol{R}} \langle i\boldsymbol{0}|\, e^{i(\boldsymbol{k}'-\boldsymbol{k})\cdot\hat{\boldsymbol{r}}}\, |j\boldsymbol{R}\rangle \\
&= \sum_{\boldsymbol{R}} e^{i\boldsymbol{k}\cdot\boldsymbol{R}} \langle i\boldsymbol{0}|\, [1 + i(\boldsymbol{k}'-\boldsymbol{k})\cdot\hat{\boldsymbol{r}}]\, |j\boldsymbol{R}\rangle
\end{aligned} \tag{10}
$$

In a low-energy subspace described by basis $\{|n\boldsymbol{k}\rangle\, | n \in \mathcal{G}\}$, we define $\langle \boldsymbol{r}|i\boldsymbol{R}\rangle$ as the Maximal Localized Wannier Function(MLWF). If $\mathcal{G}$ represents the entire Hilbert space, MLWF is δ-function, the eigen states of position operator. Otherwise, under the localization criterion introduced by [Marzari and Vanderbilt(1997)], $|i\boldsymbol{R}\rangle$ will be the eigen state of projected position operator in the subspace:

$$
\hat{\mathcal{P}} = \frac{V}{(2\pi)^3} \int \mathrm{d}\boldsymbol{k} \sum_n^{\mathcal{G}} |n\boldsymbol{k}\rangle \langle n\boldsymbol{k}| = \sum_{i\boldsymbol{R}} |i\boldsymbol{R}\rangle \langle i\boldsymbol{R}| \tag{11}
$$

$$
\hat{\mathcal{P}}\hat{\boldsymbol{r}}\hat{\mathcal{P}}\, |i\boldsymbol{R}\rangle = (\boldsymbol{R} + \boldsymbol{\tau}_i)\, |i\boldsymbol{R}\rangle \tag{12}
$$

then

$$
\begin{aligned}
\lim_{\boldsymbol{k}\to\boldsymbol{k}'} \langle u_{i\boldsymbol{k}'}|u_{j\boldsymbol{k}}\rangle_{uc} &= \sum_{\boldsymbol{R}} e^{i\boldsymbol{k}\cdot\boldsymbol{R}} \langle i\boldsymbol{0}| \hat{\mathcal{P}} \left[1 + i(\boldsymbol{k}' - \boldsymbol{k}) \cdot \hat{\boldsymbol{r}}\right] \hat{\mathcal{P}} |j\boldsymbol{R}\rangle \\
&= \sum_{\boldsymbol{R}} e^{i\boldsymbol{k}\cdot\boldsymbol{R}} \left[1 + i(\boldsymbol{k}' - \boldsymbol{k}) \cdot \boldsymbol{\tau}_i\right] \delta_{ij}\delta_{\boldsymbol{R}\boldsymbol{0}} \\
&= \delta_{ij} \left[1 + i(\boldsymbol{k}' - \boldsymbol{k}) \cdot \boldsymbol{\tau}_i\right] \\
&= \delta_{ij} e^{i(\boldsymbol{k}'-\boldsymbol{k})\cdot\boldsymbol{\tau}_i}
\end{aligned} \tag{13}
$$

For the band state,

$$
\lim_{\boldsymbol{k}\to\boldsymbol{k}'} \langle u_{n'\boldsymbol{k}'}|u_{n\boldsymbol{k}}\rangle_{uc} = \sum_i e^{i(\boldsymbol{k}'-\boldsymbol{k})\cdot\boldsymbol{\tau}_i} U_{in'}^{\boldsymbol{k}'*} U_{in}^{\boldsymbol{k}} \tag{14}
$$

So we can use $U'^{\boldsymbol{k}}_{in} = e^{-i\boldsymbol{k}\cdot\boldsymbol{\tau}_i} U^{\boldsymbol{k}}_{in}$ to represent $|u_{nk}\rangle$, their scalar product give the same result

$$
\sum_i U'^{\boldsymbol{k}'*}_{in'} U'^{\boldsymbol{k}}_{in} = \sum_i e^{i(\boldsymbol{k}'-\boldsymbol{k})\cdot\boldsymbol{\tau}_i} U_{in'}^{\boldsymbol{k}'*} U_{in}^{\boldsymbol{k}} \tag{15}
$$

Acctually, the $U'^{\boldsymbol{k}}_{in}$ is the eigen vector of Hamiltonian under atomic guage.

2.3 Finite case

Our above derivation we presented is for the case where the system is infinite. In this section, we will give some definitions in the case where the system is finite with periodic boundary condition. For Bloch states:

$$
\begin{gathered}
\text{Orthonormality: } \langle m\boldsymbol{k}|n\boldsymbol{k}'\rangle = \delta_{mn}\delta_{\boldsymbol{k}\boldsymbol{k}'} \\
\text{Completeness: } \hat{\mathcal{I}} = \sum_{n\boldsymbol{k}} |n\boldsymbol{k}\rangle \langle n\boldsymbol{k}|
\end{gathered} \tag{16}
$$

For Wannier states:

$$
\begin{gathered}
|i\boldsymbol{k}\rangle = \frac{1}{\sqrt{N}} \sum_{\boldsymbol{R}} e^{i\boldsymbol{k}\cdot\boldsymbol{R}} |i\boldsymbol{R}\rangle \,, \; |i\boldsymbol{R}\rangle = \frac{1}{\sqrt{N}} \sum_{\boldsymbol{k}} e^{-i\boldsymbol{k}\cdot\boldsymbol{R}} |i\boldsymbol{k}\rangle \\
\text{Orthonormality: } \langle i\boldsymbol{R}|j\boldsymbol{R}'\rangle = \delta_{ij}\delta_{\boldsymbol{R}\boldsymbol{R}'} \\
\text{Completeness: } \hat{\mathcal{I}} = \sum_{i\boldsymbol{R}} |i\boldsymbol{R}\rangle \langle i\boldsymbol{R}|
\end{gathered} \tag{17}
$$

2.4 Topology

3 Excitonic Model

3.1 BSE based on electronic wannier basis

In this section, we will start from the Bethe-Salpeter equation(BSE) in a system of infinite size. The infinite perspective can help us to understand the interaction clearly.

3.1.1 Excitonic Bloch state

Single excitonic bloch state can be expressed as

$$|\alpha\boldsymbol{q}\rangle = \frac{V}{(2\pi)^3}\int \mathrm{d}\boldsymbol{k}\sum_{vc}\phi_{vc}^{\alpha\boldsymbol{q}}(\boldsymbol{k})\left|\psi_{c\boldsymbol{k}+\boldsymbol{q}}^{e}\right\rangle\left|\psi_{v\boldsymbol{k}}^{h}\right\rangle = \frac{V}{(2\pi)^3}\int \mathrm{d}\boldsymbol{k}\sum_{vc}\phi_{vc}^{\alpha\boldsymbol{q}}(\boldsymbol{k})\left|vc\boldsymbol{k},\boldsymbol{q}\right\rangle \tag{18}$$

It's easy to get

$$\begin{aligned}
\langle vc\boldsymbol{k},\boldsymbol{q}|vc\boldsymbol{k}',\boldsymbol{q}'\rangle &= \frac{(2\pi)^6}{V^2}\delta_{vv'}\delta_{cc'}\delta(\boldsymbol{k}-\boldsymbol{k}')\delta(\boldsymbol{q}-\boldsymbol{q}')\\
\langle\alpha\boldsymbol{q}|\beta\boldsymbol{q}'\rangle &= \frac{(2\pi)^3}{V}\delta_{\alpha\beta}\delta(\boldsymbol{q}-\boldsymbol{q}')\\
\frac{V}{(2\pi)^3}\int \mathrm{d}\boldsymbol{k}\sum_{vc}\phi_{vc}^{\alpha\boldsymbol{q}*}(\boldsymbol{k})\phi_{vc}^{\beta\boldsymbol{q}}(\boldsymbol{k}) &= \delta_{\alpha\beta}
\end{aligned} \tag{19}$$

3.1.2 BSE

Under Tamm-Dancoff approximation (TDA), the Bethe-Salpeter equation(BSE) for exciton in a infinite system is

$$(E_{c\boldsymbol{k}+\boldsymbol{q}} - E_{v\boldsymbol{k}})\phi_{vc}^{\alpha\boldsymbol{q}}(\boldsymbol{k}) + \frac{V^2}{(2\pi)^6}\iint \mathrm{d}\boldsymbol{q}'\mathrm{d}\boldsymbol{k}'\sum_{v'c'}K_{vc,v'c'}(\boldsymbol{q},\boldsymbol{k},\boldsymbol{q}',\boldsymbol{k}')\phi_{v'c'}^{\alpha\boldsymbol{q}'}(\boldsymbol{k}') = E_{\alpha\boldsymbol{q}}\phi_{vc}^{\alpha\boldsymbol{q}}(\boldsymbol{k}) \tag{20}$$

where

$$\begin{aligned}
K_{vc,v'c'} &= K_{vcv'c'}^{d} + K_{vcv'c'}^{x}\\
K_{vcv'c'}^{d}(\boldsymbol{q},\boldsymbol{k},\boldsymbol{q}',\boldsymbol{k}') &= -\left\langle c\boldsymbol{k}+\boldsymbol{q}; v'\boldsymbol{k}'\left|W\right|v\boldsymbol{k}; c'\boldsymbol{k}'+\boldsymbol{q}'\right\rangle\\
K_{vcv'c'}^{x}(\boldsymbol{q},\boldsymbol{k},\boldsymbol{q}',\boldsymbol{k}') &= \left\langle c\boldsymbol{k}+\boldsymbol{q}; v'\boldsymbol{k}'\left|V\right|c'\boldsymbol{k}'+\boldsymbol{q}'; v\boldsymbol{k}\right\rangle
\end{aligned} \tag{21}$$

Here we define

$$\left\langle i;j\left|F\right|k;l\right\rangle = \iint \mathrm{d}\boldsymbol{r}\mathrm{d}\boldsymbol{r}'\psi_i^*(\boldsymbol{r})\psi_j^*(\boldsymbol{r}')F(\boldsymbol{r},\boldsymbol{r}')\psi_k(\boldsymbol{r}')\psi_l(\boldsymbol{r}) \tag{22}$$

Obviously we have $K_{vc,v'c'} \propto \frac{(2\pi)^3}{V}\delta(\boldsymbol{q}-\boldsymbol{q}')$, which is consistent with the conservation of excitonic momentum.

In a finite system with periodic boundary condition, eq. (20) simply becomes

$$(E_{c\boldsymbol{k}+\boldsymbol{q}} - E_{v\boldsymbol{k}})A_{vc\boldsymbol{k}}^{\alpha\boldsymbol{q}} + \sum_{v'c'\boldsymbol{k}'}K_{vc\boldsymbol{k},v'c'\boldsymbol{k}'}^{\boldsymbol{q}}A_{v'c'\boldsymbol{k}'}^{\alpha\boldsymbol{q}} = E_{\alpha\boldsymbol{q}}A_{vc\boldsymbol{k}}^{\alpha\boldsymbol{q}} \tag{23}$$

This is used for practical calculation. We can catch the details by replacing the definition of electronic wave function and the substitution of summation and integration. With electronic wannier functions, we can see the explicit process.

We can expand the Kernal terms with electronic wannier functions:

$$\begin{aligned}
K^{d}_{vcv'c'}(\boldsymbol{q},\boldsymbol{k},\boldsymbol{q}',\boldsymbol{k}') &= -\sum_{ijkl} U^{\boldsymbol{k}+\boldsymbol{q}*}_{ic} U^{\boldsymbol{k}'*}_{jv'} U^{\boldsymbol{k}}_{kv} U^{\boldsymbol{k}'+\boldsymbol{q}'}_{lc'} \left\langle i\boldsymbol{k}+\boldsymbol{q}; j\boldsymbol{k}' \left| W \right| k\boldsymbol{k}; l\boldsymbol{k}'+\boldsymbol{q}' \right\rangle \\
&= -\sum_{ijkl} U^{\boldsymbol{k}+\boldsymbol{q}*}_{ic} U^{\boldsymbol{k}'*}_{jv'} U^{\boldsymbol{k}}_{kv} U^{\boldsymbol{k}'+\boldsymbol{q}'}_{lc'} \sum_{\{\boldsymbol{R}\}} e^{-i(\boldsymbol{k}+\boldsymbol{q})\cdot\boldsymbol{R}_1} e^{-i\boldsymbol{k}'\cdot\boldsymbol{R}_2} e^{i\boldsymbol{k}\cdot\boldsymbol{R}_3} e^{i(\boldsymbol{k}'+\boldsymbol{q}')\cdot\boldsymbol{R}_4} \left\langle i\boldsymbol{R}_1; j\boldsymbol{R}_2 \left| W \right| k\boldsymbol{R}_3; l\boldsymbol{R}_4 \right\rangle \\
&= -\sum_{ijkl} U^{\boldsymbol{k}+\boldsymbol{q}*}_{ic} U^{\boldsymbol{k}'*}_{jv'} U^{\boldsymbol{k}}_{kv} U^{\boldsymbol{k}'+\boldsymbol{q}'}_{lc'} \sum_{\{\boldsymbol{R}\}} e^{-i(\boldsymbol{k}+\boldsymbol{q})\cdot\boldsymbol{R}_1} e^{-i\boldsymbol{k}'\cdot\boldsymbol{R}_2} e^{i\boldsymbol{k}\cdot\boldsymbol{R}_3} e^{i(\boldsymbol{k}'+\boldsymbol{q}')\cdot\boldsymbol{R}_4} W_{i\boldsymbol{R}_1,j\boldsymbol{R}_2,k\boldsymbol{R}_3,l\boldsymbol{R}_4} \\
&= -\sum_{ijkl} U^{\boldsymbol{k}+\boldsymbol{q}*}_{ic} U^{\boldsymbol{k}'*}_{jv'} U^{\boldsymbol{k}}_{kv} U^{\boldsymbol{k}'+\boldsymbol{q}'}_{lc'} \sum_{\boldsymbol{R}} e^{i(\boldsymbol{q}'-\boldsymbol{q})\cdot\boldsymbol{R}} \sum_{\boldsymbol{R}_1\boldsymbol{R}_2\boldsymbol{R}_3} e^{-i\boldsymbol{k}'\cdot\boldsymbol{R}_1} e^{i\boldsymbol{k}\cdot\boldsymbol{R}_2} e^{i(\boldsymbol{k}'+\boldsymbol{q}')\cdot\boldsymbol{R}_3} W_{i\boldsymbol{0},j\boldsymbol{R}_1,k\boldsymbol{R}_2,l\boldsymbol{R}_3} \\
&= -\frac{(2\pi)^3}{V}\delta(\boldsymbol{q}'-\boldsymbol{q}) K^{d\,\boldsymbol{q}}_{vcv'c'}(\boldsymbol{k},\boldsymbol{k}')
\end{aligned}$$

$$K^{d\,\boldsymbol{q}}_{vcv'c'}(\boldsymbol{k},\boldsymbol{k}') = \sum_{ijkl} U^{\boldsymbol{k}+\boldsymbol{q}*}_{ic} U^{\boldsymbol{k}'*}_{jv'} U^{\boldsymbol{k}}_{kv} U^{\boldsymbol{k}'+\boldsymbol{q}}_{lc'} \sum_{\boldsymbol{R}_1\boldsymbol{R}_2\boldsymbol{R}_3} e^{-i\boldsymbol{k}'\cdot\boldsymbol{R}_1} e^{i\boldsymbol{k}\cdot\boldsymbol{R}_2} e^{i(\boldsymbol{k}'+\boldsymbol{q})\cdot\boldsymbol{R}_3} W_{i\boldsymbol{0},j\boldsymbol{R}_1,k\boldsymbol{R}_2,l\boldsymbol{R}_3} \tag{24}$$

$$\begin{aligned}
K^{x}_{vcv'c'}(\boldsymbol{q},\boldsymbol{k},\boldsymbol{q}',\boldsymbol{k}') &= \sum_{ijkl} U^{\boldsymbol{k}+\boldsymbol{q}*}_{ic} U^{\boldsymbol{k}'*}_{jv'} U^{\boldsymbol{k}'+\boldsymbol{q}'}_{kc'} U^{\boldsymbol{k}}_{lv} \left\langle i\boldsymbol{k}+\boldsymbol{q}; j\boldsymbol{k}' \left| V \right| k\boldsymbol{k}'+\boldsymbol{q}'; l\boldsymbol{k} \right\rangle \\
&= \sum_{ijkl} U^{\boldsymbol{k}+\boldsymbol{q}*}_{ic} U^{\boldsymbol{k}'*}_{jv'} U^{\boldsymbol{k}'+\boldsymbol{q}'}_{kc'} U^{\boldsymbol{k}}_{lv} \sum_{\{\boldsymbol{R}\}} e^{-i(\boldsymbol{k}+\boldsymbol{q})\cdot\boldsymbol{R}_1} e^{-i\boldsymbol{k}'\cdot\boldsymbol{R}_2} e^{i(\boldsymbol{k}'+\boldsymbol{q}')\cdot\boldsymbol{R}_3} e^{i\boldsymbol{k}\cdot\boldsymbol{R}_4} \left\langle i\boldsymbol{R}_1; j\boldsymbol{R}_2 \left| V \right| k\boldsymbol{R}_3; l\boldsymbol{R}_4 \right\rangle \\
&= \sum_{ijkl} U^{\boldsymbol{k}+\boldsymbol{q}*}_{ic} U^{\boldsymbol{k}'*}_{jv'} U^{\boldsymbol{k}'+\boldsymbol{q}'}_{kc'} U^{\boldsymbol{k}}_{lv} \sum_{\{\boldsymbol{R}\}} e^{-i(\boldsymbol{k}+\boldsymbol{q})\cdot\boldsymbol{R}_1} e^{-i\boldsymbol{k}'\cdot\boldsymbol{R}_2} e^{i(\boldsymbol{k}'+\boldsymbol{q}')\cdot\boldsymbol{R}_3} e^{i\boldsymbol{k}\cdot\boldsymbol{R}_4} V_{i\boldsymbol{R}_1,j\boldsymbol{R}_2,k\boldsymbol{R}_3,l\boldsymbol{R}_4} \\
&= \sum_{ijkl} U^{\boldsymbol{k}+\boldsymbol{q}*}_{ic} U^{\boldsymbol{k}'*}_{jv'} U^{\boldsymbol{k}'+\boldsymbol{q}'}_{kc'} U^{\boldsymbol{k}}_{lv} \sum_{\boldsymbol{R}} e^{i(\boldsymbol{q}'-\boldsymbol{q})\cdot\boldsymbol{R}} \sum_{\boldsymbol{R}_1\boldsymbol{R}_2\boldsymbol{R}_3} e^{-i\boldsymbol{k}'\cdot\boldsymbol{R}_1} e^{i(\boldsymbol{k}'+\boldsymbol{q}')\cdot\boldsymbol{R}_2} e^{i\boldsymbol{k}\cdot\boldsymbol{R}_3} V_{i\boldsymbol{0},j\boldsymbol{R}_1,k\boldsymbol{R}_2,l\boldsymbol{R}_3} \\
&= \frac{(2\pi)^3}{V}\delta(\boldsymbol{q}'-\boldsymbol{q}) K^{x\,\boldsymbol{q}}_{vcv'c'}(\boldsymbol{k},\boldsymbol{k}')
\end{aligned}$$

$$K^{x\,\boldsymbol{q}}_{vcv'c'}(\boldsymbol{k},\boldsymbol{k}') = \sum_{ijkl} U^{\boldsymbol{k}+\boldsymbol{q}*}_{ic} U^{\boldsymbol{k}'*}_{jv'} U^{\boldsymbol{k}'+\boldsymbol{q}}_{kc'} U^{\boldsymbol{k}}_{lv} \sum_{\boldsymbol{R}_1\boldsymbol{R}_2\boldsymbol{R}_3} e^{-i\boldsymbol{k}'\cdot\boldsymbol{R}_1} e^{i(\boldsymbol{k}'+\boldsymbol{q})\cdot\boldsymbol{R}_2} e^{i\boldsymbol{k}\cdot\boldsymbol{R}_3} V_{i\boldsymbol{0},j\boldsymbol{R}_1,k\boldsymbol{R}_2,l\boldsymbol{R}_3} \tag{25}$$

The Bethe-Salpeter equation becomes

$$(E_{c\boldsymbol{k}+\boldsymbol{q}} - E_{v\boldsymbol{k}})\phi^{\alpha\boldsymbol{q}}_{vc}(\boldsymbol{k}) + \frac{V}{(2\pi)^3}\int \mathrm{d}\boldsymbol{k}' \sum_{v'c'} K^{\boldsymbol{q}}_{vc,v'c'}(\boldsymbol{k},\boldsymbol{k}')\phi^{\alpha\boldsymbol{q}}_{v'c'}(\boldsymbol{k}') = E_{\alpha\boldsymbol{q}}\phi^{\alpha\boldsymbol{q}}_{vc}(\boldsymbol{k}) \tag{26}$$

For practical calculation, the continuous integration with respect to $\boldsymbol{k}$ has to be replaced by a summation of discrete grid in Brillouion Zone. Actually this is the sampling scheme to calculate an integral in mathematics. Let we define

$$\begin{gathered}
\frac{V}{(2\pi)^3}\int \mathrm{d}\boldsymbol{k} \sum_{vc} \phi^{\alpha\boldsymbol{q}*}_{vc}(\boldsymbol{k})\phi^{\beta\boldsymbol{q}}_{vc}(\boldsymbol{k}) \approx \sum_{vc\boldsymbol{k}} \frac{V_{\boldsymbol{k}}}{V_{BZ}} \phi^{\alpha\boldsymbol{q}*}_{vc}(\boldsymbol{k})\phi^{\beta\boldsymbol{q}}_{vc}(\boldsymbol{k}) = \sum_{vc\boldsymbol{k}} A^{\alpha\boldsymbol{q}*}_{vc\boldsymbol{k}} A^{\beta\boldsymbol{q}}_{vc\boldsymbol{k}} = \delta_{\alpha\beta} \\
A^{\alpha\boldsymbol{q}}_{vc\boldsymbol{k}} = \sqrt{\frac{V_{\boldsymbol{k}}}{V_{BZ}}}\phi^{\alpha\boldsymbol{q}}_{vc}(\boldsymbol{k})
\end{gathered} \tag{27}$$

$$\begin{gathered}
(E_{c\boldsymbol{k}+\boldsymbol{q}} - E_{v\boldsymbol{k}})\sqrt{\frac{V_{\boldsymbol{k}}}{V_{BZ}}}\phi^{\alpha\boldsymbol{q}}_{vc}(\boldsymbol{k}) + \sum_{v'c'\boldsymbol{k}'} \sqrt{\frac{V_{\boldsymbol{k}}}{V_{BZ}}} K^{\boldsymbol{q}}_{vc,v'c'}(\boldsymbol{k},\boldsymbol{k}') \sqrt{\frac{V_{\boldsymbol{k}'}}{V_{BZ}}} \sqrt{\frac{V_{\boldsymbol{k}'}}{V_{BZ}}} \phi^{\alpha\boldsymbol{q}}_{v'c'}(\boldsymbol{k}') = E_{\alpha\boldsymbol{q}} \sqrt{\frac{V_{\boldsymbol{k}}}{V_{BZ}}}\phi^{\alpha\boldsymbol{q}}_{vc}(\boldsymbol{k}) \\
\Rightarrow (E_{c\boldsymbol{k}+\boldsymbol{q}} - E_{v\boldsymbol{k}})A^{\alpha\boldsymbol{q}}_{vc\boldsymbol{k}} + \sum_{v'c'\boldsymbol{k}'} K^{\boldsymbol{q}}_{vc\boldsymbol{k},v'c'\boldsymbol{k}'} A^{\alpha\boldsymbol{q}}_{v'c'\boldsymbol{k}'} = E_{\alpha\boldsymbol{q}} A^{\alpha\boldsymbol{q}}_{vc\boldsymbol{k}} \\
K^{\boldsymbol{q}}_{vc\boldsymbol{k},v'c'\boldsymbol{k}'} = \sqrt{\frac{V_{\boldsymbol{k}}}{V_{BZ}}} K^{\boldsymbol{q}}_{vc,v'c'}(\boldsymbol{k},\boldsymbol{k}') \sqrt{\frac{V_{\boldsymbol{k}'}}{V_{BZ}}}
\end{gathered} \tag{28}$$

The weights $\sqrt{\frac{V_{\boldsymbol{k}}}{V_{BZ}}}$ is useful when using a group of irreducible points in Brillouion Zone. Usually, we select an MonkhorstPack grid as the sampling scheme in the BZ. When we perform the calculation using the entire k-grid (that is, the reducible k-points), we have $\sqrt{\frac{V_{\boldsymbol{k}}}{V_{BZ}}} = \frac{1}{\sqrt{N}}$, where N represents the number of sampling points. In this situation we have $K^{\boldsymbol{q}}_{vc\boldsymbol{k},v'c'\boldsymbol{k}'} = \frac{1}{N} K^{\boldsymbol{q}}_{vc,v'c'}(\boldsymbol{k},\boldsymbol{k}')$.

3.1.3 Kernal under UJ approximation

The electron-hole interaction kernal under electronic basis have been demonstrated at eq. (24) and eq. (25). If we already get the hopping terms, we only need the interaction terms between wannier functions to calculate exciton state. The interaction terms may be complicated, but we have confirmed that only keeping direct-terms and exchange-terms is a good approximation for most system with SU2 symmetry.

If we only keep the direct term and the exchange term,

$$\begin{aligned} W_{i\boldsymbol{0},j\boldsymbol{R}_1,k\boldsymbol{R}_2,l\boldsymbol{R}_3} &= \delta_{il}\delta_{jk}\delta_{\boldsymbol{R}_3\boldsymbol{0}}\delta_{\boldsymbol{R}_1\boldsymbol{R}_2} W_{i\boldsymbol{0},j\boldsymbol{R}} + \delta_{ik}\delta_{jl}\delta_{\boldsymbol{R}_2\boldsymbol{0}}\delta_{\boldsymbol{R}_1\boldsymbol{R}_3} J^1_{i\boldsymbol{0},j\boldsymbol{R}} + \delta_{ij}\delta_{kl}\delta_{\boldsymbol{R}_1\boldsymbol{0}}\delta_{\boldsymbol{R}_2\boldsymbol{R}_3} J^2_{i\boldsymbol{0},k\boldsymbol{R}} \\ V_{i\boldsymbol{0},j\boldsymbol{R}_1,k\boldsymbol{R}_2,l\boldsymbol{R}_3} &= \delta_{il}\delta_{jk}\delta_{\boldsymbol{R}_3\boldsymbol{0}}\delta_{\boldsymbol{R}_1\boldsymbol{R}_2} V_{i\boldsymbol{0},j\boldsymbol{R}} + \delta_{ik}\delta_{jl}\delta_{\boldsymbol{R}_2\boldsymbol{0}}\delta_{\boldsymbol{R}_1\boldsymbol{R}_3} X^1_{i\boldsymbol{0},j\boldsymbol{R}} + \delta_{ij}\delta_{kl}\delta_{\boldsymbol{R}_1\boldsymbol{0}}\delta_{\boldsymbol{R}_2\boldsymbol{R}_3} X^2_{i\boldsymbol{0},k\boldsymbol{R}} \end{aligned} \tag{29}$$

With the definition $F_{ij}(\boldsymbol{k}) = \sum_{\boldsymbol{R}} e^{i\boldsymbol{k}\cdot\boldsymbol{R}} F_{i\boldsymbol{0},j\boldsymbol{R}}$, we can simplify the Kernal to

$$\begin{aligned} K^{d\,\boldsymbol{q}}_{vc\boldsymbol{k}v'c'\boldsymbol{k}'} = -\frac{1}{N}\sum_{ij}\Big[& U^{\boldsymbol{k}+\boldsymbol{q}*}_{ic} U^{\boldsymbol{k}'*}_{jv'} U^{\boldsymbol{k}}_{jv} U^{\boldsymbol{k}'+\boldsymbol{q}}_{ic'} W_{ij}(\boldsymbol{k}-\boldsymbol{k}') \\ & + U^{\boldsymbol{k}+\boldsymbol{q}*}_{ic} U^{\boldsymbol{k}'*}_{jv'} U^{\boldsymbol{k}}_{iv} U^{\boldsymbol{k}'+\boldsymbol{q}}_{jc'} J^1_{ij}(\boldsymbol{q}) + U^{\boldsymbol{k}+\boldsymbol{q}*}_{ic} U^{\boldsymbol{k}'*}_{iv'} U^{\boldsymbol{k}}_{jv} U^{\boldsymbol{k}'+\boldsymbol{q}}_{jc'} J^2_{ij}(\boldsymbol{k}+\boldsymbol{k}'+\boldsymbol{q})\Big] \end{aligned} \tag{30}$$

$$\begin{aligned} K^{x\,\boldsymbol{q}}_{vc\boldsymbol{k}v'c'\boldsymbol{k}'} = \frac{1}{N}\sum_{ij}\Big[& U^{\boldsymbol{k}+\boldsymbol{q}*}_{ic} U^{\boldsymbol{k}'*}_{jv'} U^{\boldsymbol{k}'+\boldsymbol{q}}_{jc'} U^{\boldsymbol{k}}_{iv} V_{ij}(\boldsymbol{q}) \\ & + U^{\boldsymbol{k}+\boldsymbol{q}*}_{ic} U^{\boldsymbol{k}'*}_{jv'} U^{\boldsymbol{k}'+\boldsymbol{q}}_{ic'} U^{\boldsymbol{k}}_{jv} X^1_{ij}(\boldsymbol{k}-\boldsymbol{k}') + U^{\boldsymbol{k}+\boldsymbol{q}*}_{ic} U^{\boldsymbol{k}'*}_{iv'} U^{\boldsymbol{k}'+\boldsymbol{q}}_{jc'} U^{\boldsymbol{k}}_{jv} X^2_{ij}(\boldsymbol{k}+\boldsymbol{k}'+\boldsymbol{q})\Big] \end{aligned} \tag{31}$$

Here we emphasize that, direct term $W_{ij}(\boldsymbol{k})$ or $V_{ij}(\boldsymbol{k})$ contains the interaction over infinite distances due to the $\frac{1}{r}$ decay trend of direct term. Only in the infinite case we can see the summation of $\boldsymbol{R}$ contains the entire space clearly. This is why we start from the BSE in a system with infinite size.

3.1.4 Handle the divergency in Kernal

3.2 Excitonic Band state

3.2.1 Bloch state $|\alpha\boldsymbol{q}\rangle$

Actually, we have give the Bloch states of exciton in section 3.1.1 for infinite case:

$$\begin{aligned} |\alpha\boldsymbol{q}\rangle &= \frac{V}{(2\pi)^3}\int \mathrm{d}\boldsymbol{k}\sum_{vc}\phi^{\alpha\boldsymbol{q}}_{vc}(\boldsymbol{k})\,|vc\boldsymbol{k},\boldsymbol{q}\rangle \\ \langle vc\boldsymbol{k},\boldsymbol{q}|vc\boldsymbol{k}',\boldsymbol{q}'\rangle &= \frac{(2\pi)^6}{V^2}\delta_{vv'}\delta_{cc'}\delta(\boldsymbol{k}-\boldsymbol{k}')\delta(\boldsymbol{q}-\boldsymbol{q}') \\ \langle\alpha\boldsymbol{q}|\beta\boldsymbol{q}'\rangle &= \frac{(2\pi)^3}{V}\delta_{\alpha\beta}\delta(\boldsymbol{q}-\boldsymbol{q}') \\ \frac{V}{(2\pi)^3}\int \mathrm{d}\boldsymbol{k}&\sum_{vc}\phi^{\alpha\boldsymbol{q}*}_{vc}(\boldsymbol{k})\phi^{\beta\boldsymbol{q}}_{vc}(\boldsymbol{k}) = \delta_{\alpha\beta} \end{aligned} \tag{32}$$

Similarly we can give the definition for the approximation of finite case:

$$
\begin{aligned}
|\alpha\boldsymbol{q}\rangle &= \sum_{vc\boldsymbol{k}} A^{\alpha\boldsymbol{q}}_{vc\boldsymbol{k}} |vc\boldsymbol{k},\boldsymbol{q}\rangle \\
\langle vc\boldsymbol{k},\boldsymbol{q}|vc\boldsymbol{k}',\boldsymbol{q}'\rangle &= \frac{(2\pi)^3}{V}\delta_{vv'}\delta_{cc'}\delta_{\boldsymbol{k},\boldsymbol{k}'}\delta(\boldsymbol{q}-\boldsymbol{q}') \\
\langle \alpha\boldsymbol{q}|\beta\boldsymbol{q}'\rangle &= \frac{(2\pi)^3}{V}\delta_{\alpha\beta}\delta(\boldsymbol{q}-\boldsymbol{q}') \\
\sum_{vc\boldsymbol{k}} A^{\alpha\boldsymbol{q}*}_{vc\boldsymbol{k}} A^{\beta\boldsymbol{q}}_{vc\boldsymbol{k}} &= \delta_{\alpha\beta}
\end{aligned}
\tag{33}
$$

Note we retain $\frac{(2\pi)^3}{V}\delta(\boldsymbol{q}-\boldsymbol{q}')$ because we regard the finite case as the approximation of infinite case. This notion allows us to calculate the excitonic states of a random $\boldsymbol{q}$ by solving BSE on a finite grid in BZ numerically.

3.2.2 $|u_{\alpha\boldsymbol{q}}\rangle = e^{-i\boldsymbol{q}\cdot\hat{\boldsymbol{r}}_0}|\alpha\boldsymbol{q}\rangle$

Exciton have two spacial varialbes: $\boldsymbol{r}_e$ and $\boldsymbol{r}_h$. We can define λ as the weight to calculate the center position of exciton:

$$
\begin{aligned}
\boldsymbol{r}_0 &= (1-\lambda)\boldsymbol{r}_e + \lambda\boldsymbol{r}_h,\ \boldsymbol{r} = \boldsymbol{r}_e - \boldsymbol{r}_h \\
\boldsymbol{r}_e &= \boldsymbol{r}_0 + \lambda\boldsymbol{r},\ \boldsymbol{r}_h = \boldsymbol{r}_0 - (1-\lambda)\boldsymbol{r}
\end{aligned}
\tag{34}
$$

Define:

$$
\begin{aligned}
\left|u^{\lambda}_{\alpha\boldsymbol{q}}\right\rangle &= e^{-i\boldsymbol{q}\cdot\hat{\boldsymbol{r}}_0}|\alpha\boldsymbol{q}\rangle = \frac{V}{(2\pi)^3}\int \mathrm{d}\boldsymbol{k}\sum_{vc}\phi^{\alpha\boldsymbol{q}}_{vc}(\boldsymbol{k})e^{-i\boldsymbol{q}\cdot\hat{\boldsymbol{r}}_0}|vc\boldsymbol{k},\boldsymbol{q}\rangle = \frac{V}{(2\pi)^3}\int \mathrm{d}\boldsymbol{k}\sum_{vc}\phi^{\alpha\boldsymbol{q}}_{vc}(\boldsymbol{k})\left|u^{\lambda\boldsymbol{q}}_{vc\boldsymbol{k}}\right\rangle \\
\left|u^{\lambda\boldsymbol{q}}_{vc\boldsymbol{k}}\right\rangle &= e^{-i\boldsymbol{q}\cdot\hat{\boldsymbol{r}}_0}|vc\boldsymbol{k},\boldsymbol{q}\rangle = e^{-i\boldsymbol{q}\cdot\hat{\boldsymbol{r}}_0}\left|\psi^{e}_{c\boldsymbol{k}+\boldsymbol{q}}\right\rangle\left|\psi^{h}_{v\boldsymbol{k}}\right\rangle = e^{i(\boldsymbol{k}+\lambda\boldsymbol{q})\cdot\hat{\boldsymbol{r}}}\left|u^{e}_{c\boldsymbol{k}+\boldsymbol{q}}\right\rangle\left|u^{h}_{v\boldsymbol{k}}\right\rangle
\end{aligned}
\tag{35}
$$

Under translation operator $\hat{T}_{\boldsymbol{R}}$, we have

$$
\begin{aligned}
\hat{T}_{\boldsymbol{R}}|vc\boldsymbol{k},\boldsymbol{q}\rangle = e^{i(\boldsymbol{k}+\boldsymbol{q})\cdot\boldsymbol{R}}e^{-i\boldsymbol{k}\cdot\boldsymbol{R}}|vc\boldsymbol{k},\boldsymbol{q}\rangle = e^{i\boldsymbol{q}\cdot\boldsymbol{R}}|vc\boldsymbol{k},\boldsymbol{q}\rangle &\Rightarrow \hat{T}_{\boldsymbol{R}}|\alpha\boldsymbol{q}\rangle = e^{i\boldsymbol{q}\cdot\boldsymbol{R}}|\alpha\boldsymbol{q}\rangle \\
\hat{T}_{\boldsymbol{R}}\left|u^{\lambda}_{\alpha\boldsymbol{q}}\right\rangle = e^{-i\boldsymbol{q}\cdot(\hat{\boldsymbol{r}}_0+\boldsymbol{R})}e^{i\boldsymbol{q}\cdot\boldsymbol{R}}|\alpha\boldsymbol{q}\rangle &= \left|u^{\lambda}_{\alpha\boldsymbol{q}}\right\rangle
\end{aligned}
\tag{36}
$$

This prove that $\left|u^{\lambda}_{\alpha\boldsymbol{q}}\right\rangle$ is a periodic function defined in an unitcell.

Similarly, we need to calculate the inner product of $\left\langle u^{\lambda}_{\alpha\boldsymbol{q}}\middle|u^{\lambda}_{\beta\boldsymbol{q}'}\right\rangle$ in an unitcell, where $\boldsymbol{q}$ and $\boldsymbol{q}'$ is adjacent. We try to analyze the inner product of basis $\left|u^{\lambda\boldsymbol{q}}_{vc\boldsymbol{k}}\right\rangle$ firstly.

$$
\begin{aligned}
\lim_{\boldsymbol{q}\to\boldsymbol{q}'}\left\langle u^{\lambda\boldsymbol{q}}_{vc\boldsymbol{k}}\middle|u^{\lambda\boldsymbol{q}'}_{v'c'\boldsymbol{k}'}\right\rangle_{uc} &= \frac{1}{\sum_{\boldsymbol{R}}}\left\langle u^{e}_{c\boldsymbol{k}+\boldsymbol{q}}\right|\left\langle u^{h}_{v\boldsymbol{k}}\right| e^{i(\boldsymbol{k}'+\lambda\boldsymbol{q}'-\boldsymbol{k}-\lambda\boldsymbol{q})\cdot\hat{\boldsymbol{r}}}\left|u^{e}_{c'\boldsymbol{k}'+\boldsymbol{q}'}\right\rangle\left|u^{h}_{v'\boldsymbol{k}'}\right\rangle \\
&= \frac{1}{\sum_{\boldsymbol{R}}}\left\langle u^{e}_{c\boldsymbol{k}+\boldsymbol{q}}\right| e^{i(\boldsymbol{k}'+\lambda\boldsymbol{q}'-\boldsymbol{k}-\lambda\boldsymbol{q})\cdot\hat{\boldsymbol{r}}_e}\left|u^{e}_{c'\boldsymbol{k}'+\boldsymbol{q}'}\right\rangle\left\langle u^{h}_{v\boldsymbol{k}}\right| e^{i(\boldsymbol{k}'+\lambda\boldsymbol{q}'-\boldsymbol{k}-\lambda\boldsymbol{q})\cdot\hat{\boldsymbol{r}}_h}\left|u^{h}_{v'\boldsymbol{k}'}\right\rangle \\
&= \frac{1}{\sum_{\boldsymbol{R}}}\sum_{\boldsymbol{R}} e^{i(\boldsymbol{k}'+\lambda\boldsymbol{q}'-\boldsymbol{k}-\lambda\boldsymbol{q})\cdot\boldsymbol{R}}\left\langle u^{e}_{c\boldsymbol{k}+\boldsymbol{q}}\right| e^{i(\boldsymbol{k}'+\lambda\boldsymbol{q}'-\boldsymbol{k}-\lambda\boldsymbol{q})\cdot\hat{\boldsymbol{r}}_e}\left|u^{e}_{c'\boldsymbol{k}'+\boldsymbol{q}'}\right\rangle_{uc}\left\langle u^{h}_{v\boldsymbol{k}}\right| e^{i(\boldsymbol{k}'+\lambda\boldsymbol{q}'-\boldsymbol{k}-\lambda\boldsymbol{q})\cdot\hat{\boldsymbol{r}}_h}\left|u^{h}_{v'\boldsymbol{k}'}\right\rangle \\
&= \frac{1}{\sum_{\boldsymbol{R}}}\frac{(2\pi)^3}{V}\delta(\boldsymbol{k}'+\lambda\boldsymbol{q}'-\boldsymbol{k}-\lambda\boldsymbol{q})\left\langle u^{e}_{c\boldsymbol{k}+\boldsymbol{q}}\middle|u^{e}_{c'\boldsymbol{k}'+\boldsymbol{q}'}\right\rangle_{uc}\left\langle u^{h}_{v\boldsymbol{k}}\middle|u^{h}_{v'\boldsymbol{k}'}\right\rangle \\
&= \frac{(2\pi)^3}{V}\delta(\boldsymbol{k}'+\lambda\boldsymbol{q}'-\boldsymbol{k}-\lambda\boldsymbol{q})\left\langle u^{e}_{c\boldsymbol{k}+\boldsymbol{q}}\middle|u^{e}_{c'\boldsymbol{k}'+\boldsymbol{q}'}\right\rangle_{uc}\left\langle u^{h}_{v\boldsymbol{k}}\middle|u^{h}_{v'\boldsymbol{k}'}\right\rangle_{uc}
\end{aligned}
\tag{37}
$$

Here, the δ-function means we have to perform the conditional summation of $A^{\alpha\boldsymbol{q}}_{vc\boldsymbol{k}}$ based on the specific values of $\boldsymbol{k}$ and $\boldsymbol{q}$ in numerical calculation. It's a little bit complicated. But we find another method to give a concrete form representing $|u_{\alpha\boldsymbol{q}}\rangle$:

$$
\begin{aligned}
\lim_{\boldsymbol{q}\to\boldsymbol{q}'}\left\langle u^{\lambda\boldsymbol{q}}_{vc\boldsymbol{k}}\middle|u^{\lambda\boldsymbol{q}'}_{v'c'\boldsymbol{k}'}\right\rangle_{uc} &= \frac{1}{\sum_{\boldsymbol{R}}}\left\langle\psi^e_{c\boldsymbol{k}+\boldsymbol{q}}\right|\left\langle\psi^h_{v\boldsymbol{k}}\right| e^{i(\boldsymbol{q}-\boldsymbol{q}')\cdot[(1-\lambda)\hat{\boldsymbol{r}}_e+\lambda\hat{\boldsymbol{r}}_h]}\left|\psi^e_{c'\boldsymbol{k}'+\boldsymbol{q}'}\right\rangle\left|\psi^h_{v'\boldsymbol{k}'}\right\rangle \\
&= \frac{1}{\sum_{\boldsymbol{R}}}\left\langle\psi^e_{c\boldsymbol{k}+\boldsymbol{q}}\right| e^{i(1-\lambda)(\boldsymbol{q}-\boldsymbol{q}')\cdot\hat{\boldsymbol{r}}_e}\left|\psi^e_{c'\boldsymbol{k}'+\boldsymbol{q}'}\right\rangle\left\langle\psi^h_{v\boldsymbol{k}}\right| e^{i\lambda(\boldsymbol{q}-\boldsymbol{q}')\cdot\hat{\boldsymbol{r}}_h}\left|\psi^h_{v'\boldsymbol{k}'}\right\rangle \\
&= \frac{1}{\sum_{\boldsymbol{R}}}\sum_{ij\boldsymbol{R}_e\boldsymbol{R}_h}\sum_{i'j'\boldsymbol{R}'_e\boldsymbol{R}'_h} U^{\boldsymbol{k}+\boldsymbol{q}*}_{ic}U^{\boldsymbol{k}}_{jv}U^{\boldsymbol{k}'+\boldsymbol{q}'}_{i'c'}U^{\boldsymbol{k}'*}_{j'v'}e^{-i(\boldsymbol{k}+\boldsymbol{q})\cdot\boldsymbol{R}_e}e^{i\boldsymbol{k}\cdot\boldsymbol{R}_h}e^{i(\boldsymbol{k}'+\boldsymbol{q}')\cdot\boldsymbol{R}'_e}e^{-i\boldsymbol{k}'\cdot\boldsymbol{R}'_h} \\
&\qquad\times\left\langle\psi^e_{i\boldsymbol{R}_e}\right| e^{i(1-\lambda)(\boldsymbol{q}-\boldsymbol{q}')\cdot\hat{\boldsymbol{r}}_e}\left|\psi^e_{i'\boldsymbol{R}'_e}\right\rangle\left\langle\psi^h_{j\boldsymbol{R}_h}\right| e^{i\lambda(\boldsymbol{q}-\boldsymbol{q}')\cdot\hat{\boldsymbol{r}}_h}\left|\psi^h_{j'\boldsymbol{R}'_h}\right\rangle
\end{aligned}
\tag{38}
$$

If electronic wannier function is MLWF, we have

$$
\lim_{\boldsymbol{k}\to 0}\left\langle\psi_{i\boldsymbol{R}}\right| e^{i\boldsymbol{k}\cdot\hat{\boldsymbol{r}}}\left|\psi_{i'\boldsymbol{R}'}\right\rangle = \delta_{ii'}\delta_{\boldsymbol{R}\boldsymbol{R}'}e^{i\boldsymbol{k}\cdot(\boldsymbol{R}+\boldsymbol{\tau}_i)}
\tag{39}
$$

then

$$
\begin{aligned}
\lim_{\boldsymbol{q}\to\boldsymbol{q}'}\left\langle u^{\lambda\boldsymbol{q}}_{vc\boldsymbol{k}}\middle|u^{\lambda\boldsymbol{q}'}_{v'c'\boldsymbol{k}'}\right\rangle_{uc} &= \frac{1}{\sum_{\boldsymbol{R}}}\sum_{ij\boldsymbol{R}_e\boldsymbol{R}_h} U^{\boldsymbol{k}+\boldsymbol{q}*}_{ic}U^{\boldsymbol{k}}_{jv}U^{\boldsymbol{k}'+\boldsymbol{q}'}_{ic'}U^{\boldsymbol{k}'*}_{jv'}e^{-i(\boldsymbol{k}+\boldsymbol{q})\cdot\boldsymbol{R}_e}e^{i\boldsymbol{k}\cdot\boldsymbol{R}_h}e^{i(\boldsymbol{k}'+\boldsymbol{q}')\cdot\boldsymbol{R}_e}e^{-i\boldsymbol{k}'\cdot\boldsymbol{R}_h} \\
&\qquad\times e^{i(1-\lambda)(\boldsymbol{q}-\boldsymbol{q}')\cdot(\boldsymbol{R}_e+\boldsymbol{\tau}_i)}e^{i\lambda(\boldsymbol{q}-\boldsymbol{q}')\cdot(\boldsymbol{R}_h+\boldsymbol{\tau}_j)} \\
&= \frac{1}{\sum_{\boldsymbol{R}}}\sum_{ij\boldsymbol{R}_e\boldsymbol{R}_h} U^{\boldsymbol{k}+\boldsymbol{q}*}_{ic}U^{\boldsymbol{k}}_{jv}U^{\boldsymbol{k}'+\boldsymbol{q}'}_{ic'}U^{\boldsymbol{k}'*}_{jv'}e^{i(\boldsymbol{k}-\boldsymbol{k}')\cdot(\boldsymbol{R}_h-\boldsymbol{R}_e)}e^{i\lambda(\boldsymbol{q}-\boldsymbol{q}')\cdot(\boldsymbol{R}_h-\boldsymbol{R}_e)} \\
&\qquad\times e^{i(\boldsymbol{q}-\boldsymbol{q}')\cdot[(1-\lambda)\boldsymbol{\tau}_i+\lambda\boldsymbol{\tau}_j]} \\
&= \frac{1}{\sum_{\boldsymbol{R}}}\sum_{\boldsymbol{R}_0}\sum_{ij\boldsymbol{R}} U^{\boldsymbol{k}+\boldsymbol{q}*}_{ic}U^{\boldsymbol{k}}_{jv}U^{\boldsymbol{k}'+\boldsymbol{q}'}_{ic'}U^{\boldsymbol{k}'*}_{jv'}e^{i(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{R}}e^{i\lambda(\boldsymbol{q}-\boldsymbol{q}')\cdot\boldsymbol{R}}e^{i(\boldsymbol{q}-\boldsymbol{q}')\cdot[(1-\lambda)\boldsymbol{\tau}_i+\lambda\boldsymbol{\tau}_j]} \\
&= \sum_{ij\boldsymbol{R}} U^{\boldsymbol{k}+\boldsymbol{q}*}_{ic}U^{\boldsymbol{k}}_{jv}U^{\boldsymbol{k}'+\boldsymbol{q}'}_{ic'}U^{\boldsymbol{k}'*}_{jv'}e^{i(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{R}}e^{i\lambda(\boldsymbol{q}-\boldsymbol{q}')\cdot\boldsymbol{R}}e^{i(\boldsymbol{q}-\boldsymbol{q}')\cdot[(1-\lambda)\boldsymbol{\tau}_i+\lambda\boldsymbol{\tau}_j]} \\
&= \sum_{ij\boldsymbol{R}} A^{vc\boldsymbol{k},\boldsymbol{q}*}_{ij\boldsymbol{R}}A^{v'c'\boldsymbol{k}',\boldsymbol{q}'}_{ij\boldsymbol{R}}
\end{aligned}
\tag{40}
$$

where

$$
\begin{aligned}
A^{vc\boldsymbol{k},\boldsymbol{q}}_{ij\boldsymbol{R}} &= U^{\boldsymbol{k}+\boldsymbol{q}}_{ic}U^{\boldsymbol{k}*}_{jv}e^{-i(\boldsymbol{k}+\lambda\boldsymbol{q})\cdot\boldsymbol{R}}e^{-i\boldsymbol{q}\cdot[(1-\lambda)\boldsymbol{\tau}_i+\lambda\boldsymbol{\tau}_j]} \\
\sum_{ij\boldsymbol{R}} A^{vc\boldsymbol{k},\boldsymbol{q}*}_{ij\boldsymbol{R}}A^{vc\boldsymbol{k},\boldsymbol{q}}_{ij\boldsymbol{R}} &= 1
\end{aligned}
\tag{41}
$$

We can use $A^{vc\boldsymbol{k}}_{ij\boldsymbol{R}}$ to represent $\left|u^{\lambda\boldsymbol{q}}_{vc\boldsymbol{k}}\right\rangle$. For excitonic band state we have

$$
\begin{aligned}
A^{\alpha\boldsymbol{q}}_{ij\boldsymbol{R}} &= e^{-i\lambda\boldsymbol{q}\cdot\boldsymbol{R}}e^{-i\boldsymbol{q}\cdot[(1-\lambda)\boldsymbol{\tau}_i+\lambda\boldsymbol{\tau}_j]}\frac{V}{(2\pi)^3}\int \mathrm{d}\boldsymbol{k}\sum_{vc}\phi^{\alpha\boldsymbol{q}}_{vc}(\boldsymbol{k})U^{\boldsymbol{k}+\boldsymbol{q}}_{ic}U^{\boldsymbol{k}*}_{jv}e^{-i\boldsymbol{k}\cdot\boldsymbol{R}} \\
&\approx e^{-i\lambda\boldsymbol{q}\cdot\boldsymbol{R}}e^{-i\boldsymbol{q}\cdot[(1-\lambda)\boldsymbol{\tau}_i+\lambda\boldsymbol{\tau}_j]}\frac{1}{\sqrt{N}}\sum_{vc\boldsymbol{k}}A^{\alpha\boldsymbol{q}}_{vc\boldsymbol{k}}U^{\boldsymbol{k}+\boldsymbol{q}}_{ic}U^{\boldsymbol{k}*}_{jv}e^{-i\boldsymbol{k}\cdot\boldsymbol{R}}
\end{aligned}
\tag{42}
$$

There is only one thing need to be noticed. $\boldsymbol{R}$ actually represents the distance between the cells where electron or hole locates. The bigger $|\boldsymbol{R}|$ is, the smaller $|A^{\alpha\boldsymbol{q}}_{ij\boldsymbol{R}}|$ is. In infinite case, the value of $\boldsymbol{R}$ is infinitely numerous. But in finite case, $\boldsymbol{R}$ has only N possible values. Here N is the number of kpoints and represents the size of system. So we have to ensure that N is large enough so that $A^{\alpha\boldsymbol{q}}_{ij\boldsymbol{R}}$ includes all the sufficiently large components.

3.3 Excitonic Topology

This subsection only give the simple deduce, then refer other paper.

3.3.1 Berry Connection

$$
\begin{aligned}
\mathcal{A}^{0}_{\alpha\beta}(q) &= \frac{V}{(2\pi)^3}\int \mathrm{d}k \sum_{vc}\left[i\phi^{\alpha\boldsymbol{q}*}_{vc}(\boldsymbol{k})\boldsymbol{\nabla}_{\boldsymbol{q}}\phi^{\beta\boldsymbol{q}}_{vc}(\boldsymbol{k}) + \sum_{c'} A^{\alpha q*}_{vck}A^{\beta q}_{vc'k}A^{ele}_{cc'}(k+q)\right] \\
A^{1}_{\alpha\beta}(q) &= \frac{V}{(2\pi)^3}\int \mathrm{d}k \sum_{vc}\left[iA^{\alpha q*}_{vck}\nabla_q A^{\beta q}_{vck} - iA^{\alpha q*}_{vck}\nabla_k A^{\beta q}_{vck} + \sum_{v'} A^{\alpha q*}_{vck}A^{\beta q}_{v'ck}A^{ele}_{v'v}(k)\right]
\end{aligned}
\tag{43}
$$

$$
A^{\lambda}_{\alpha\beta}(q) = i\left\langle u^{\lambda}_{\alpha q}\middle|\nabla_q\middle|u^{\lambda}_{\beta q}\right\rangle_{uc} = (1-\lambda)A^{0}_{\alpha\beta}(q) + \lambda A^{1}_{\alpha\beta}(q) \tag{44}
$$

3.3.2 Berry Curvature

4 Direct term between wannier functions

The direct term between wannier functions is defined as

$$\begin{aligned}
V_{ij}(\boldsymbol{k}) &= \sum_{\boldsymbol{R}} e^{i\boldsymbol{k}\cdot\boldsymbol{R}} V_{i\boldsymbol{0},j\boldsymbol{R}} \\
V_{i\boldsymbol{0},j\boldsymbol{R}} &= \iint \mathrm{d}\boldsymbol{r}\mathrm{d}\boldsymbol{r}' \left|\psi_{i\boldsymbol{0}}(\boldsymbol{r})\right|^2 V(\boldsymbol{r},\boldsymbol{r}') \left|\psi_{j\boldsymbol{R}}(\boldsymbol{r}')\right|^2
\end{aligned} \tag{45}$$

4.1 Long-range part

With the Coulomb potential generated by a charge of Gaussian distribution (54), we can expand $V_{ij}(\boldsymbol{k})$ as

$$\begin{aligned}
V_{ij}(\boldsymbol{k}) &= \sum_{\boldsymbol{R}} e^{i\boldsymbol{k}\cdot\boldsymbol{R}} V_{i\boldsymbol{0},j\boldsymbol{R}} \\
&= \sum_{\boldsymbol{R}} e^{i\boldsymbol{k}\cdot\boldsymbol{R}} \left[V_{i\boldsymbol{0},j\boldsymbol{R}} - \phi(\boldsymbol{R}+\boldsymbol{\tau}_j-\boldsymbol{\tau}_i)\right] + \sum_{\boldsymbol{R}} e^{i\boldsymbol{k}\cdot\boldsymbol{R}} \phi(\boldsymbol{R}+\boldsymbol{\tau}_j-\boldsymbol{\tau}_i) \\
&= V_{ij}^{sr}(\boldsymbol{k}) + \phi_{ij}(\boldsymbol{k})
\end{aligned} \tag{46}$$

The components of short-range term $V_{ij}^{sr}(\boldsymbol{k})$ decay to 0 rapidly, so that $V_{ij}^{sr}(\boldsymbol{k})$ can be calculated in real space. With fourier transformation (**??**), the long-range term can be expressed

In this section, we will give a analytical form of the long range part of direct term. We use the screened interaction as example, the naked direct term is similar. The direct terms between wannier functions is defined as

$$W_{i\boldsymbol{0},j\boldsymbol{R}} = \iint \mathrm{d}\boldsymbol{r}\mathrm{d}\boldsymbol{r}' \left|\psi_{i\boldsymbol{0}}(\boldsymbol{r})\right|^2 W(\boldsymbol{r},\boldsymbol{r}') \left|\psi_{j\boldsymbol{R}}(\boldsymbol{r}')\right|^2 \tag{47}$$

When $\boldsymbol{R}$ is large enough, $W_{i\boldsymbol{0},j\boldsymbol{R}}$ is approximate to $W(\boldsymbol{R}+\boldsymbol{\tau}_j-\boldsymbol{\tau}_i)$. The components of short-range term $W_{ij}^{sr}(\boldsymbol{k})$ decay to 0 rapidly, so that $W_{ij}^{sr}(\boldsymbol{k})$ can be calculated in real space. With Poisson summation, the long-range term can be expressed

$$W_{ij}^{lr}(\boldsymbol{k}) = \frac{1}{V} \sum_{\boldsymbol{G}} W(\boldsymbol{k}+\boldsymbol{G}) e^{-i(\boldsymbol{k}+\boldsymbol{G})\cdot(\boldsymbol{\tau}_j-\boldsymbol{\tau}_i)} \tag{48}$$

The number of parameters that we can provide is a finite set, and we

4.2 Mirror Correction

A Fourier transform of a sum function

Define a function with summation:

$$F(\mathbf{r}) = \sum_{\mathbf{R}} f(\mathbf{r} + \mathbf{R}) \tag{49}$$

3D case:

$$\begin{aligned}
F(\mathbf{r}) = F(\mathbf{r} + \mathbf{R}) = \sum_{\mathbf{k}} F(\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{r}},\ e^{i\mathbf{k}\cdot\mathbf{R}} = 1 \\
F(\mathbf{k}) &= \frac{1}{\Omega} \int_{\Omega} \mathrm{d}\mathbf{r}\, F(\mathbf{r}) e^{-i\mathbf{k}\cdot\mathbf{r}} \\
&= \frac{1}{\Omega} \int_{\Omega} \mathrm{d}\mathbf{r} \sum_{\mathbf{R}} f(\mathbf{r} + \mathbf{R}) e^{-i\mathbf{k}\cdot(\mathbf{r}+\mathbf{R})} \\
&= \frac{1}{\Omega} \int \mathrm{d}\mathbf{r}\, f(\mathbf{r}) e^{-i\mathbf{k}\cdot\mathbf{r}} \\
&= \frac{1}{\Omega} f(\mathbf{k})
\end{aligned} \tag{50}$$

2D case:

$$\begin{aligned}
F(\mathbf{r}) = F(x + R_x, y + R_y, z) = \sum_{\mathbf{k}} F(k_x, k_y, z) e^{i(k_x x + k_y y)},\ e^{i(k_x R_x + k_y R_y)} = 1 \\
F(k_x, k_y, z) &= \frac{1}{S} \int_S \mathrm{d}x\mathrm{d}y F(\mathbf{r}) e^{-i(k_x x + k_y y)} \\
&= \frac{1}{S} \int_S \mathrm{d}x\mathrm{d}y \sum_{R_x R_y} f(\mathbf{r} + \mathbf{R}) e^{-i\mathbf{k}\cdot(\mathbf{r}+\mathbf{R})} \\
&= \frac{1}{S} \int \mathrm{d}x\mathrm{d}y f(\mathbf{r}) e^{-i\mathbf{k}\cdot\mathbf{r}} \\
&= \frac{1}{S} f(\mathbf{k}, z)
\end{aligned} \tag{51}$$

1D case:

$$\begin{aligned}
F(\mathbf{r}) = F(x + R_x, y, z) = \sum_{\mathbf{k}} F(k_x, y, z) e^{ik_x x},\ e^{ik_x R_x} = 1 \\
F(k_x, y, z) &= \frac{1}{L} \int_L \mathrm{d}x F(\mathbf{r}) e^{-ik_x x} \\
&= \frac{1}{L} \int_L \mathrm{d}x \sum_{R_x} f(\mathbf{r} + \mathbf{R}) e^{-i\mathbf{k}\cdot(\mathbf{r}+\mathbf{R})} \\
&= \frac{1}{L} \int \mathrm{d}x f(\mathbf{r}) e^{-ik_x x} \\
&= \frac{1}{L} f(k_x, y, z)
\end{aligned} \tag{52}$$

B Gaussian potential

Gaussian distribution:

$$G(\boldsymbol{r}) = \left(\frac{\alpha}{\sqrt{\pi}}\right)^3 e^{-\alpha^2|\boldsymbol{r}|^2} \tag{53}$$

Coulomb potential generated by a charge of Gaussian distribution(omit $\frac{e^2}{4\pi\epsilon_0}$):

$$\begin{aligned} \nabla^2\phi(\boldsymbol{r}) = -4\pi G(\boldsymbol{r}) \Rightarrow \phi(\boldsymbol{r}) = \frac{erf(\alpha|\boldsymbol{r}|)}{|\boldsymbol{r}|} \\ \phi(0) = \frac{2\alpha}{\sqrt{\pi}},\ erf(x) = \frac{2}{\sqrt{\pi}}\int_0^x e^{-t^2}\mathrm{d}t \end{aligned} \tag{54}$$

Features: long-range bahavior is is proportional to $\frac{1}{r}$.

$$\lim_{|r|\to\infty}\phi(\boldsymbol{r}) = \frac{1}{|\boldsymbol{r}|} \tag{55}$$

B.1 Fourier transformation

3D case:

$$\phi(\boldsymbol{k}) = \int \mathrm{d}\boldsymbol{r}\phi(\boldsymbol{r})e^{-ikr} = \frac{4\pi}{\boldsymbol{k}^2}e^{-\frac{\boldsymbol{k}^2}{4\alpha^2}} \tag{56}$$

2D case:

$$\phi(k_x, k_y, z) = \int \mathrm{d}x\mathrm{d}y\phi(\boldsymbol{r})e^{-i(k_x x + k_y y)} = \frac{\pi}{|\boldsymbol{k}|}\left[e^{|\boldsymbol{k}|z}erfc(\frac{|\boldsymbol{k}|}{2\alpha} + \alpha z) + e^{-|\boldsymbol{k}|z}erfc(\frac{|\boldsymbol{k}|}{2\alpha} - \alpha z)\right] \tag{57}$$

1D case: To be continued.

References