WannierExcitonModel.jl - Theory

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Contents

Chapter 1

Introduction

This is the Physical background for WannierExcitonModel.jl.

Chapter 2

Tight Binding Model

2.1 Poison summation

Finite case:

$$\begin{aligned}\sum_{\boldsymbol{R}} e^{i(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{R}} &= N\delta_{\boldsymbol{k}\boldsymbol{k}'} \\ \sum_{\boldsymbol{k}} e^{i\boldsymbol{k}\cdot(\boldsymbol{R}-\boldsymbol{R}')} &= N\delta_{\boldsymbol{R}\boldsymbol{R}'}\end{aligned} \tag{2.1}$$

Infinite case:

$$\begin{aligned}\sum_{\boldsymbol{R}} e^{i(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{R}} &= \frac{(2\pi)^3}{V}\delta(\boldsymbol{k}-\boldsymbol{k}') \\ \frac{V}{(2\pi)^3}\int \mathrm{d}\boldsymbol{k} e^{i\boldsymbol{k}\cdot(\boldsymbol{R}-\boldsymbol{R}')} &= \delta_{\boldsymbol{R}\boldsymbol{R}'}\end{aligned} \tag{2.2}$$

2.2 Band state

For the case where the system is infinite, we define

$$\begin{aligned}\text{Orthonormality: } \left\langle m\boldsymbol{k}\middle|n\boldsymbol{k}'\right\rangle &= \frac{(2\pi)^3}{V}\delta_{mn}\delta(\boldsymbol{k}-\boldsymbol{k}') \\ \text{Completeness: } \hat{\mathcal{I}} &= \frac{V}{(2\pi)^3}\int \mathrm{d}\boldsymbol{k}\sum_n \left|n\boldsymbol{k}\right\rangle\left\langle n\boldsymbol{k}\right|\end{aligned} \tag{2.3}$$

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

$$\begin{aligned}\left|n\boldsymbol{k}\right\rangle = \sum_i U_{in}^{\boldsymbol{k}}\left|i\boldsymbol{k}\right\rangle,\ \left|i\boldsymbol{k}\right\rangle &= \sum_n U_{in}^{\boldsymbol{k}*}\left|n\boldsymbol{k}\right\rangle \\ \text{Orthonormality: } \left\langle i\boldsymbol{k}\middle|j\boldsymbol{k}'\right\rangle &= \frac{(2\pi)^3}{V}\delta_{ij}\delta(\boldsymbol{k}-\boldsymbol{k}') \\ \text{Completeness: } \hat{\mathcal{I}} &= \frac{V}{(2\pi)^3}\int \mathrm{d}\boldsymbol{k}\sum_i \left|i\boldsymbol{k}\right\rangle\left\langle i\boldsymbol{k}\right|\end{aligned} \tag{2.4}$$

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

$$
\begin{gathered}
|i\boldsymbol{k}\rangle = \sum_{\boldsymbol{R}} e^{i\boldsymbol{k}\cdot\boldsymbol{R}} |i\boldsymbol{R}\rangle\,,\ |i\boldsymbol{R}\rangle = \frac{V}{(2\pi)^3}\int \mathrm{d}\boldsymbol{k} e^{-i\boldsymbol{k}\cdot\boldsymbol{R}} |i\boldsymbol{k}\rangle \\
\text{Orthonormality: } \left\langle i\boldsymbol{R} \middle| j\boldsymbol{R}' \right\rangle = \delta_{ij}\delta_{\boldsymbol{R}\boldsymbol{R}'} \\
\text{Completeness: } \hat{\mathcal{I}} = \sum_{i\boldsymbol{R}} |i\boldsymbol{R}\rangle \langle i\boldsymbol{R}|
\end{gathered}
\tag{2.5}
$$

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

In the low-energy subspace described by basis $\{|n\boldsymbol{k}\rangle\, | n \in \mathcal{G}\}$, we can get the numerical vector form of Bloch function $|n\boldsymbol{k}\rangle$ with wannier basis.

$$
|n\boldsymbol{k}\rangle = \sum_i U_{in}^{\boldsymbol{k}} |i\boldsymbol{k}\rangle = \sum_{i\boldsymbol{R}} U_{in}^{\boldsymbol{k}} e^{i\boldsymbol{k}\cdot\boldsymbol{R}} |i\boldsymbol{R}\rangle \tag{2.6}
$$

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

$$
\begin{aligned}
\left\langle i\boldsymbol{k}' \right| H \left| n\boldsymbol{k} \right\rangle &= \sum_j U_{jn}^{\boldsymbol{k}} \sum_{\boldsymbol{R}'\boldsymbol{R}} e^{i\left(\boldsymbol{k}\cdot\boldsymbol{R}-\boldsymbol{k}'\cdot\boldsymbol{R}'\right)} \left\langle i\boldsymbol{R}' \right| H \left| j\boldsymbol{R} \right\rangle \\
&= \sum_j U_{jn}^{\boldsymbol{k}} \sum_{\boldsymbol{R}'\boldsymbol{R}} e^{i\left(\boldsymbol{k}-\boldsymbol{k}'\right)\cdot\boldsymbol{R}'} e^{i\boldsymbol{k}\cdot\left(\boldsymbol{R}-\boldsymbol{R}'\right)} \langle i\boldsymbol{0}| H \left| j\boldsymbol{R}-\boldsymbol{R}' \right\rangle \\
&= \sum_j U_{jn}^{\boldsymbol{k}} \sum_{\boldsymbol{R}_0} e^{i\left(\boldsymbol{k}-\boldsymbol{k}'\right)\cdot\boldsymbol{R}_0} \sum_{\boldsymbol{R}} e^{i\boldsymbol{k}\cdot\boldsymbol{R}} \langle i\boldsymbol{0}| H \left| j\boldsymbol{R} \right\rangle \\
&= \frac{(2\pi)^3}{V}\delta(\boldsymbol{k}-\boldsymbol{k}') \sum_j H_{ij}^{\boldsymbol{k}} U_{jn}^{\boldsymbol{k}}
\end{aligned}
\tag{2.7}
$$

$$
\begin{aligned}
\left\langle i\boldsymbol{k}' \right| E_{n\boldsymbol{k}} \left| n\boldsymbol{k} \right\rangle &= \frac{(2\pi)^3}{V}\delta(\boldsymbol{k}-\boldsymbol{k}') E_{n\boldsymbol{k}} U_{in}^{\boldsymbol{k}} \\
&\Rightarrow \sum_j H_{ij}^{\boldsymbol{k}} U_{jn}^{\boldsymbol{k}} = E_{n\boldsymbol{k}} U_{in}^{\boldsymbol{k}}
\end{aligned}
\tag{2.8}
$$

where

$$
H_{ij}^{\boldsymbol{k}} = \sum_{\boldsymbol{R}} e^{i\boldsymbol{k}\cdot\boldsymbol{R}} \langle i\boldsymbol{0}| H \left| j\boldsymbol{R} \right\rangle \tag{2.9}
$$

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 $|n\boldsymbol{k}\rangle$.

$$
\begin{gathered}
|u_{n\boldsymbol{k}}\rangle = e^{-i\boldsymbol{k}\cdot\hat{\boldsymbol{r}}}\,|n\boldsymbol{k}\rangle = \sum_i U_{in}^{\boldsymbol{k}} e^{-i\boldsymbol{k}\cdot\hat{\boldsymbol{r}}}\,|i\boldsymbol{k}\rangle = \sum_i U_{in}^{\boldsymbol{k}}\,|u_{i\boldsymbol{k}}\rangle \\
|u_{i\boldsymbol{k}}\rangle = \sum_{\boldsymbol{R}} e^{i\boldsymbol{k}\cdot(\boldsymbol{R}-\hat{\boldsymbol{r}})}\,|i\boldsymbol{R}\rangle
\end{gathered}
\tag{2.10}
$$

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

$$
\begin{aligned}
\lim_{\boldsymbol{k}\to\boldsymbol{k}'} \langle u_{i\boldsymbol{k}'}|u_{j\boldsymbol{k}}\rangle_{uc} &= \frac{1}{\sum_{\boldsymbol{R}_0}} \langle u_{i\boldsymbol{k}'}|u_{j\boldsymbol{k}}\rangle \\
&= \frac{1}{\sum_{\boldsymbol{R}_0}} \sum_{\boldsymbol{R}'\boldsymbol{R}} e^{i\left(\boldsymbol{k}\cdot\boldsymbol{R}-\boldsymbol{k}'\cdot\boldsymbol{R}'\right)} \left\langle i\boldsymbol{R}'\right| e^{i(\boldsymbol{k}'-\boldsymbol{k})\cdot\hat{\boldsymbol{r}}} \left|j\boldsymbol{R}\right\rangle \\
&= \frac{1}{\sum_{\boldsymbol{R}_0}} \sum_{\boldsymbol{R}_0\boldsymbol{R}} e^{i\boldsymbol{k}\cdot\boldsymbol{R}} \langle i\boldsymbol{0}| e^{i(\boldsymbol{k}'-\boldsymbol{k})\cdot\hat{\boldsymbol{r}}} |j\boldsymbol{R}\rangle \\
&= \sum_{\boldsymbol{R}} e^{i\boldsymbol{k}\cdot\boldsymbol{R}} \langle i\boldsymbol{0}| \left[1+i(\boldsymbol{k}'-\boldsymbol{k})\cdot\hat{\boldsymbol{r}}\right] |j\boldsymbol{R}\rangle
\end{aligned} \tag{2.11}
$$

If $\langle \boldsymbol{r}|i\boldsymbol{R}\rangle$ is the Maximal Localized Wannier Function(MLWF), $|i\boldsymbol{R}\rangle$ will be the eigen state of projected position operator:

$$
\hat{\mathcal{P}} = \frac{V}{(2\pi)^3} \int \mathrm{d}\boldsymbol{k} \sum_{n}^{\mathcal{G}} |n\boldsymbol{k}\rangle \langle n\boldsymbol{k}| \tag{2.12}
$$

$$
\hat{\mathcal{P}}\hat{\boldsymbol{r}}\hat{\mathcal{P}} |i\boldsymbol{R}\rangle = (\boldsymbol{R}+\boldsymbol{\tau}_i) |i\boldsymbol{R}\rangle \tag{2.13}
$$

then

$$
\begin{aligned}
\lim_{\boldsymbol{k}\to\boldsymbol{k}'} \langle u_{i\boldsymbol{k}'}|u_{j\boldsymbol{k}}\rangle_{uc} &= \sum_{\boldsymbol{R}} e^{i\boldsymbol{k}\cdot\boldsymbol{R}} \langle i\boldsymbol{0}| \hat{\mathcal{P}} \left[1+i(\boldsymbol{k}'-\boldsymbol{k})\cdot\hat{\boldsymbol{r}}\right] \hat{\mathcal{P}} |j\boldsymbol{R}\rangle \\
&= \sum_{\boldsymbol{R}} e^{i\boldsymbol{k}\cdot\boldsymbol{R}} \left[1+i(\boldsymbol{k}'-\boldsymbol{k})\cdot\boldsymbol{\tau}_i\right] \delta_{ij}\delta_{\boldsymbol{R}\boldsymbol{0}} \\
&= \delta_{ij} \left[1+i(\boldsymbol{k}'-\boldsymbol{k})\cdot\boldsymbol{\tau}_i\right] \\
&= \delta_{ij} e^{i(\boldsymbol{k}'-\boldsymbol{k})\cdot\boldsymbol{\tau}_i}
\end{aligned} \tag{2.14}
$$

For the band state,

$$
\lim_{\boldsymbol{k}\to\boldsymbol{k}'} \langle u_{n'\boldsymbol{k}'}|u_{n\boldsymbol{k}}\rangle_{uc} = \sum_{i} e^{i(\boldsymbol{k}'-\boldsymbol{k})\cdot\boldsymbol{\tau}_i} U_{in'}^{\boldsymbol{k}'*} U_{in}^{\boldsymbol{k}} \tag{2.15}
$$

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

$$
\sum_{i} {U'}_{in'}^{\boldsymbol{k}'*} {U'}_{in}^{\boldsymbol{k}} = \sum_{i} e^{i(\boldsymbol{k}'-\boldsymbol{k})\cdot\boldsymbol{\tau}_i} U_{in'}^{\boldsymbol{k}'*} U_{in}^{\boldsymbol{k}} \tag{2.16}
$$

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

2.2.3 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:

$$
\begin{aligned}
\text{Orthonormality: } \left\langle m\boldsymbol{k}\middle|n\boldsymbol{k}'\right\rangle &= \delta_{mn}\delta_{\boldsymbol{k}\boldsymbol{k}'} \\
\text{Completeness: } \hat{\mathcal{I}} &= \sum_{n\boldsymbol{k}} |n\boldsymbol{k}\rangle \langle n\boldsymbol{k}|
\end{aligned} \tag{2.17}
$$

For Wannier states:

$$
\begin{aligned}
|i\boldsymbol{k}\rangle = \frac{1}{\sqrt{N}} \sum_{\boldsymbol{R}} e^{i\boldsymbol{k}\cdot\boldsymbol{R}} |i\boldsymbol{R}\rangle &, \ |i\boldsymbol{R}\rangle = \frac{1}{\sqrt{N}} \sum_{\boldsymbol{k}} e^{-i\boldsymbol{k}\cdot\boldsymbol{R}} |i\boldsymbol{k}\rangle \\
\text{Orthonormality: } \left\langle i\boldsymbol{R}\middle|j\boldsymbol{R}'\right\rangle &= \delta_{ij}\delta_{\boldsymbol{R}\boldsymbol{R}'} \\
\text{Completeness: } \hat{\mathcal{I}} &= \sum_{i\boldsymbol{R}} |i\boldsymbol{R}\rangle \langle i\boldsymbol{R}|
\end{aligned} \tag{2.18}
$$

2.3 Topology

Chapter 3

Excitonic BSE Model

3.1 BSE based on electronic wannier basis

The standard Bethe-Salpeter equation for exciton is

$$(E_{c\boldsymbol{k}+\boldsymbol{q}} - E_{v\boldsymbol{k}})A^{\alpha}_{vc}(\boldsymbol{q},\boldsymbol{k}) + \frac{V}{(2\pi)^3}\int \mathrm{d}\boldsymbol{k}'\sum_{v'c'}\left[K^{d}_{vc,v'c'}(\boldsymbol{q},\boldsymbol{k},\boldsymbol{k}') + K^{x}_{vc,v'c'}(\boldsymbol{q},\boldsymbol{k},\boldsymbol{k}')\right]A^{\alpha}_{v'c'}(\boldsymbol{q},\boldsymbol{k}') = E_{\alpha\boldsymbol{q}}A^{\alpha}_{vc}(\boldsymbol{q},\boldsymbol{k}) \tag{3.1}$$

where

$$\begin{aligned} K^{d\,\boldsymbol{q}}_{v'c'\boldsymbol{k}'vc\boldsymbol{k}} &= -\left\langle c'\boldsymbol{k}'+\boldsymbol{q}; v\boldsymbol{k}\left|W\right|v'\boldsymbol{k}'; c\boldsymbol{k}+\boldsymbol{q}\right\rangle \\ K^{x\,\boldsymbol{q}}_{v'c'\boldsymbol{k}'vc\boldsymbol{k}} &= \left\langle c'\boldsymbol{k}'+\boldsymbol{q}; v\boldsymbol{k}\left|V\right|c\boldsymbol{k}+\boldsymbol{q}; v'\boldsymbol{k}'\right\rangle \end{aligned} \tag{3.2}$$

Note here we define

$$\langle i; j\left|F\right|k; l\rangle = \iint \mathrm{d}\boldsymbol{r}\mathrm{d}\boldsymbol{r}'\psi^*_i(\boldsymbol{r})\psi^*_j(\boldsymbol{r}')F(\boldsymbol{r},\boldsymbol{r}')\psi_k(\boldsymbol{r}')\psi_l(\boldsymbol{r}) \tag{3.3}$$

Thretically, we should imagine a infinite system and $\boldsymbol{k}$ should be a continuous variable. But the BSE is mainly used to do practical calculation, which prefer a discrete form. Note a discrete grid of kpoints can be regarded as sampling grids for numerically calculating continuous integrals. This sampling perspective can help us understand the subsequent processing steps.

With electronic wannier functions, we can expand the Kernal terms as

$$\begin{aligned} K^{d\,\boldsymbol{q}}_{v'c'\boldsymbol{k}'vc\boldsymbol{k}} &= -\sum_{ijkl} U^{\boldsymbol{k}'+\boldsymbol{q}*}_{ic'}U^{\boldsymbol{k}*}_{jv}U^{\boldsymbol{k}'}_{kv'}U^{\boldsymbol{k}+\boldsymbol{q}}_{lc}\left\langle i\boldsymbol{k}'+\boldsymbol{q}; j\boldsymbol{k}\left|W\right|k\boldsymbol{k}'; l\boldsymbol{k}+\boldsymbol{q}\right\rangle \\ &= -\sum_{ijkl} U^{\boldsymbol{k}'+\boldsymbol{q}*}_{ic'}U^{\boldsymbol{k}*}_{jv}U^{\boldsymbol{k}'}_{kv'}U^{\boldsymbol{k}+\boldsymbol{q}}_{lc}\frac{1}{N^2}\sum_{\{\boldsymbol{R}\}} e^{-i(\boldsymbol{k}'+\boldsymbol{q})\cdot\boldsymbol{R}_1}e^{-i\boldsymbol{k}\cdot\boldsymbol{R}_2}e^{i\boldsymbol{k}'\cdot\boldsymbol{R}_3}e^{i(\boldsymbol{k}+\boldsymbol{q})\cdot\boldsymbol{R}_4}\left\langle i\boldsymbol{R}_1; j\boldsymbol{R}_2\left|W\right|k\boldsymbol{R}_3; l\boldsymbol{R}_4\right\rangle \\ &= -\sum_{ijkl} U^{\boldsymbol{k}'+\boldsymbol{q}*}_{ic'}U^{\boldsymbol{k}*}_{jv}U^{\boldsymbol{k}'}_{kv'}U^{\boldsymbol{k}+\boldsymbol{q}}_{lc}\frac{1}{N^2}\sum_{\{\boldsymbol{R}\}} e^{-i(\boldsymbol{k}'+\boldsymbol{q})\cdot\boldsymbol{R}_1}e^{-i\boldsymbol{k}\cdot\boldsymbol{R}_2}e^{i\boldsymbol{k}'\cdot\boldsymbol{R}_3}e^{i(\boldsymbol{k}+\boldsymbol{q})\cdot\boldsymbol{R}_4}W_{i\boldsymbol{R}_1,j\boldsymbol{R}_2,k\boldsymbol{R}_3,l\boldsymbol{R}_4} \\ &= -\sum_{ijkl} U^{\boldsymbol{k}'+\boldsymbol{q}*}_{ic'}U^{\boldsymbol{k}*}_{jv}U^{\boldsymbol{k}'}_{kv'}U^{\boldsymbol{k}+\boldsymbol{q}}_{lc}\frac{1}{N}\sum_{\boldsymbol{R}_1\boldsymbol{R}_2\boldsymbol{R}_3} e^{-i\boldsymbol{k}\cdot\boldsymbol{R}_1}e^{i\boldsymbol{k}'\cdot\boldsymbol{R}_2}e^{i(\boldsymbol{k}+\boldsymbol{q})\cdot\boldsymbol{R}_3}W_{i\boldsymbol{0},j\boldsymbol{R}_1,k\boldsymbol{R}_2,l\boldsymbol{R}_3} \end{aligned} \tag{3.4}$$

$$
\begin{aligned}
K^{x\,\boldsymbol{q}}_{v'c'\boldsymbol{k}'vc\boldsymbol{k}} &= \sum_{ijkl} U^{\boldsymbol{k}'+\boldsymbol{q}*}_{ic'} U^{\boldsymbol{k}*}_{jv} U^{\boldsymbol{k}+\boldsymbol{q}}_{kc} U^{\boldsymbol{k}'}_{lv'} \left\langle i\boldsymbol{k}'+\boldsymbol{q}; j\boldsymbol{k} \left| V \right| k\boldsymbol{k}+\boldsymbol{q}; l\boldsymbol{k}' \right\rangle \\
&= \sum_{ijkl} U^{\boldsymbol{k}'+\boldsymbol{q}*}_{ic'} U^{\boldsymbol{k}*}_{jv} U^{\boldsymbol{k}+\boldsymbol{q}}_{kc} U^{\boldsymbol{k}'}_{lv'} \frac{1}{N^2} \sum_{\{\boldsymbol{R}\}} e^{-i(\boldsymbol{k}'+\boldsymbol{q})\cdot\boldsymbol{R}_1} e^{-i\boldsymbol{k}\cdot\boldsymbol{R}_2} e^{i(\boldsymbol{k}+\boldsymbol{q})\cdot\boldsymbol{R}_3} e^{i\boldsymbol{k}'\cdot\boldsymbol{R}_4} \left\langle i\boldsymbol{R}_1; j\boldsymbol{R}_2 \left| V \right| k\boldsymbol{R}_3; l\boldsymbol{R}_4 \right\rangle \\
&= \sum_{ijkl} U^{\boldsymbol{k}'+\boldsymbol{q}*}_{ic'} U^{\boldsymbol{k}*}_{jv} U^{\boldsymbol{k}'}_{kv'} U^{\boldsymbol{k}+\boldsymbol{q}}_{lc} \frac{1}{N^2} \sum_{\{\boldsymbol{R}\}} e^{-i(\boldsymbol{k}'+\boldsymbol{q})\cdot\boldsymbol{R}_1} e^{-i\boldsymbol{k}\cdot\boldsymbol{R}_2} e^{i(\boldsymbol{k}+\boldsymbol{q})\cdot\boldsymbol{R}_3} e^{i\boldsymbol{k}'\cdot\boldsymbol{R}_4} V_{i\boldsymbol{R}_1, j\boldsymbol{R}_2, k\boldsymbol{R}_3, l\boldsymbol{R}_4} \\
&= \sum_{ijkl} U^{\boldsymbol{k}'+\boldsymbol{q}*}_{ic'} U^{\boldsymbol{k}*}_{jv} U^{\boldsymbol{k}'}_{kv'} U^{\boldsymbol{k}+\boldsymbol{q}}_{lc} \frac{1}{N} \sum_{\boldsymbol{R}_1\boldsymbol{R}_2\boldsymbol{R}_3} e^{-i\boldsymbol{k}\cdot\boldsymbol{R}_1} e^{i(\boldsymbol{k}+\boldsymbol{q})\cdot\boldsymbol{R}_2} e^{i\boldsymbol{k}'\cdot\boldsymbol{R}_3} V_{i\boldsymbol{0}, j\boldsymbol{R}_1, k\boldsymbol{R}_2, l\boldsymbol{R}_3}
\end{aligned}
\tag{3.5}
$$

3.1.1 Kernal under UJ approximation

If we only keep the direct term U and the exchange term J, we can simplify the Kernal to

3.2 Excitonic Band state

3.3 Excitonic Topology

Chapter 4

Interaction parameters between wannier functions

4.1 Direct terms

4.1.1 Mirror Correction

4.1.2 Long-range Correction

4.2 The practical calculation of Interaction parameters

Chapter 5

Appendix

5.1 Gaussian potential

Bibliography