Homework 4

Yusheng Zhao

March 5, 2023

Contents

1 Problem 1

$$\psi_k(\vec{r}) = \frac{1}{\sqrt{N}} \sum_{\vec{R}} e^{i\vec{k}\cdot\vec{R}} \phi_s(\vec{r} - \vec{R}) \tag{1}$$

$$= e^{i\vec{k}\cdot\vec{r}} \frac{1}{\sqrt{N}} \sum_{\vec{R}} e^{i\vec{k}\cdot(\vec{R}-\vec{r})} \phi_s(\vec{r} - \vec{R}) \tag{2}$$

Next we only need to show $\frac{1}{\sqrt{N}} \sum_{\vec{R}} e^{i\vec{k}\cdot(\vec{R}-\vec{r})} \phi_s(\vec{r} - \vec{R})$ is periodic in lattice vectors. Meaning that if we define $u(\vec{r}) = \frac{1}{\sqrt{N}} \sum_{\vec{R}} e^{i\vec{k}\cdot(\vec{R}-\vec{r})} \phi_s(\vec{r} - \vec{R})$, we need to have $u(\vec{r}) = u(\vec{r} + \vec{R}'$

$$\frac{1}{\sqrt{N}} \sum_{\vec{R}} e^{i\vec{k}\cdot(\vec{R}-(\vec{r}+\vec{R}'))} \phi_s((\vec{r} + \vec{R}') - \vec{R}) \tag{3}$$

$$= \frac{1}{\sqrt{N}} \sum_{\vec{R}} e^{i\vec{k}\cdot((\vec{R}-\vec{R}')-\vec{r})} \phi_s(\vec{r} - (\vec{R} - \vec{R}')) \tag{4}$$

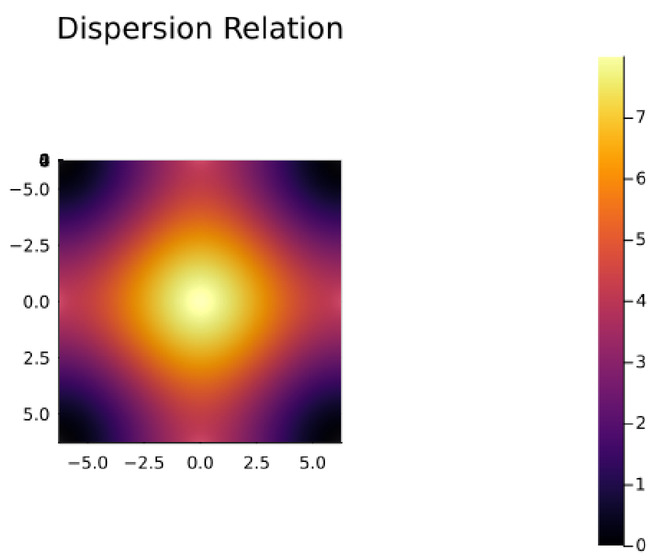
$$= \frac{1}{\sqrt{N}} \sum_{\vec{R}''} e^{i\vec{k}\cdot(\vec{R}''-\vec{r})} \phi_s(\vec{r} - \vec{R}'') \tag{5}$$

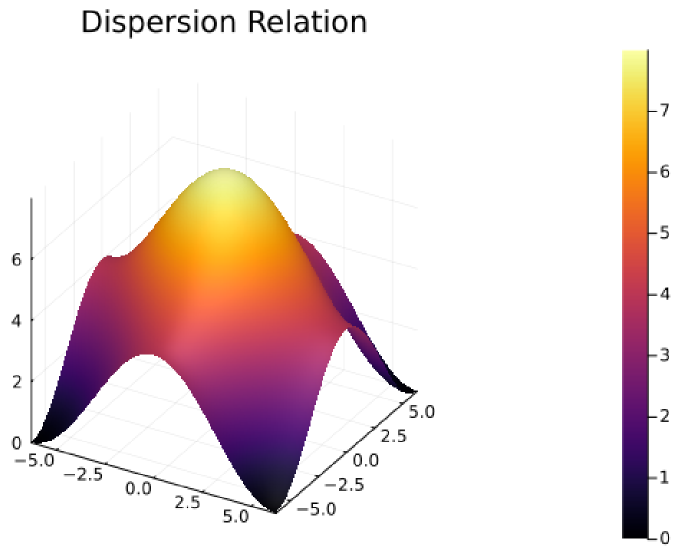
$$= \frac{1}{\sqrt{N}} \sum_{\vec{R}} e^{i\vec{k}\cdot(\vec{R}-\vec{r})} \phi_s(\vec{r} - \vec{R}) \quad \square \tag{6}$$

2 Problem 2

- Let's consider only the nearest neighbor hopping case, and make the strength $\gamma = 1eV$.
- Let the lattice size be $a = 0.5$ angstrom.
- Let's make $\int \psi^*(x) H \psi(x) dx = \epsilon = 4eV$
- $E(k_x, k_y = \epsilon + 2 * \gamma * (cos(k_x * a) + cos(k_y * a))$

```
using Plots
a = 0.5
 = 4.0
 = 1.0
kx = -/0.5:0.01:/0.5
ky = -/0.5:0.01:/0.5
E(kx,ky) =  + 2.0 *  * cos(kx*a) + 2.0 *  * cos(ky*a)
# plot(kx,ky,E,st=:surface,camera=(90,90);title="Dispersion Relation",label="E(kx,ky)")
plot(kx,ky,E,st=:surface;title="Dispersion Relation",label="E(kx,ky)")
xlabel!("kx 1/angstrom")
ylabel!("ky 1/angstrom")
zlabel!("Energy (eV)")
```




Dispersion Relation
6
4
2
0
−5.0
−2.5
0.0
2.5
5.0
5.0
2.5
0.0
−2.5
−5.0
7
6
5
4
3
2
1
0