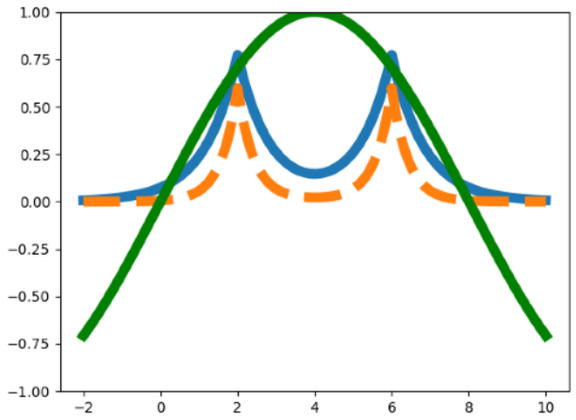
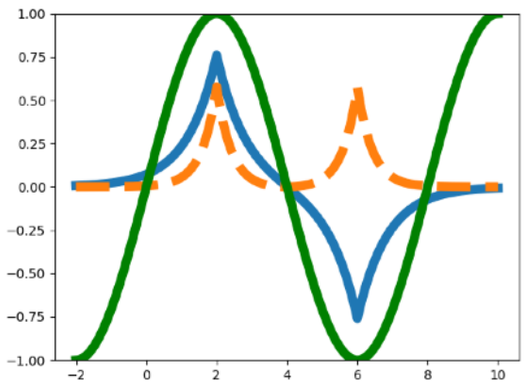
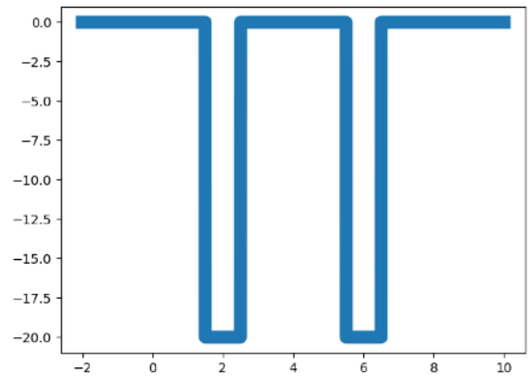
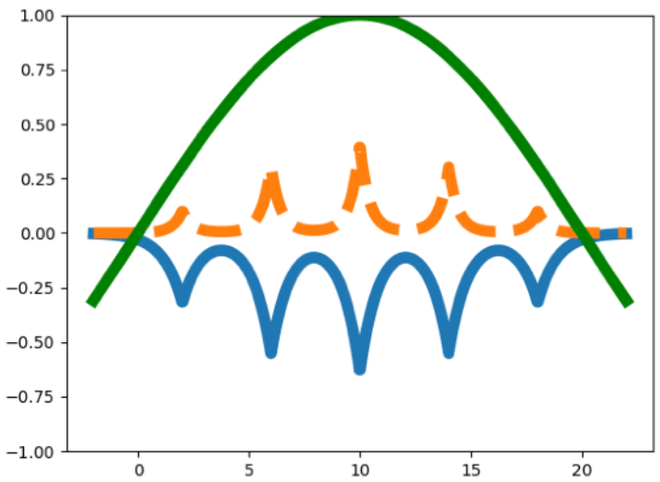
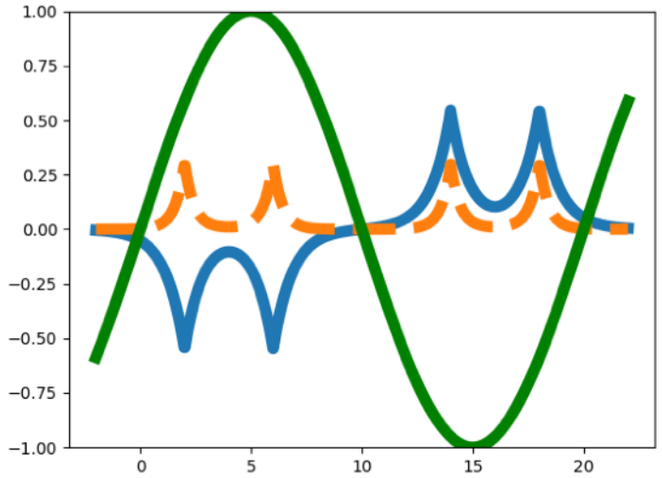

1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
−2
0
2
4
6
8
10

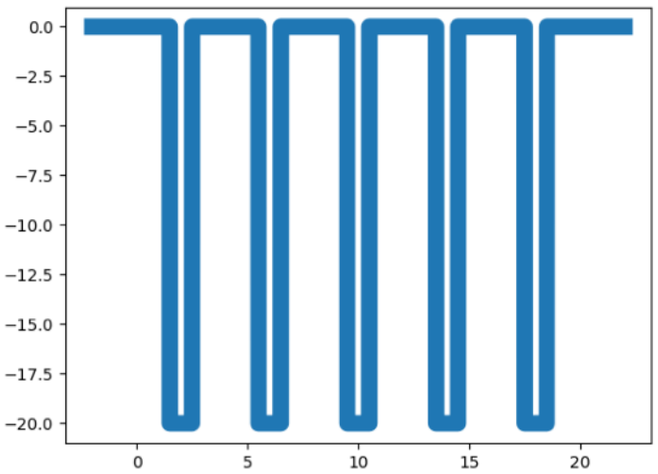

1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
−2
0
2
4
6
8
10

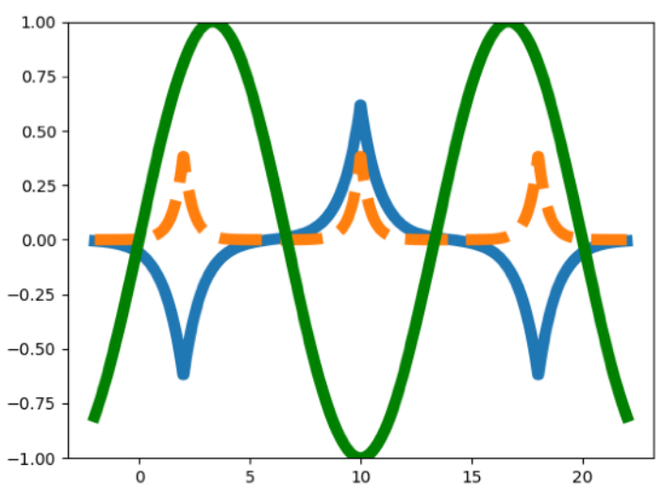

0.0
−2.5
−5.0
−7.5
−10.0
−12.5
−15.0
−17.5
−20.0
−2
0
2
4
6
8
10

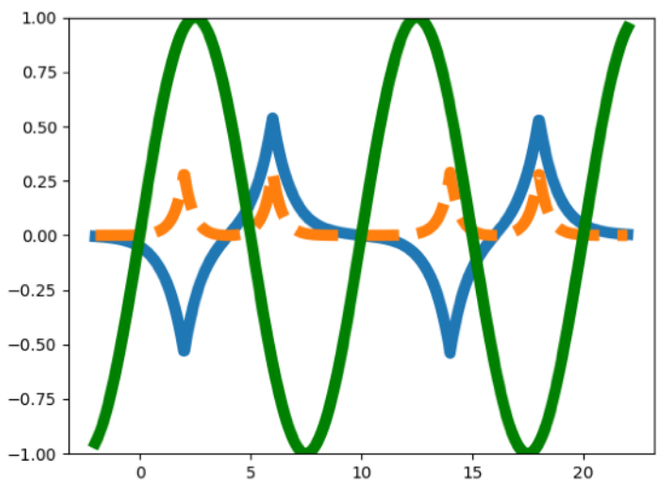
$$\Psi(x) = e^{ikx}u(x)$$

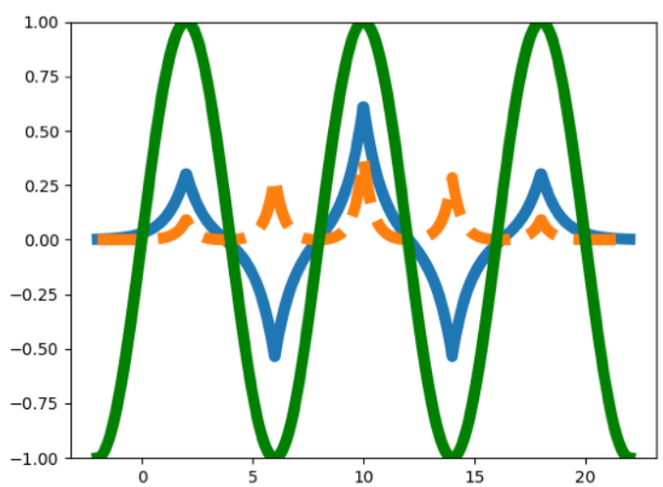

1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
0
5
10
15
20


1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
0
5
10
15
20

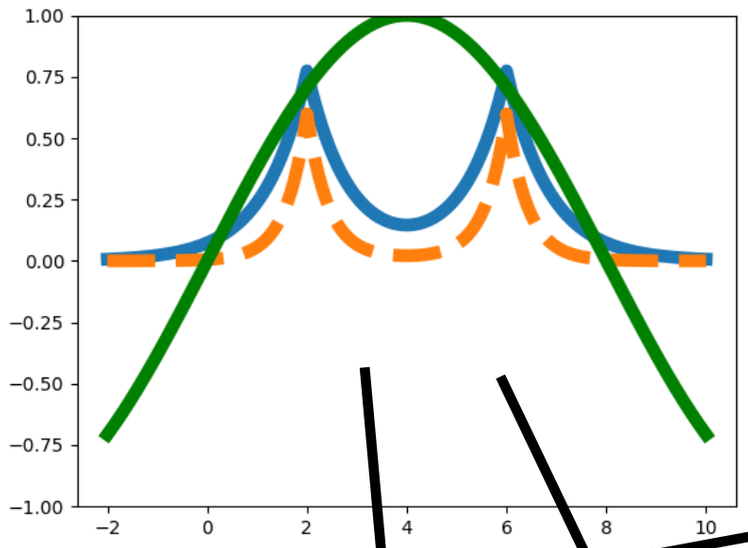

0.0
−2.5
−5.0
−7.5
−10.0
−12.5
−15.0
−17.5
−20.0
0
5
10
15
20

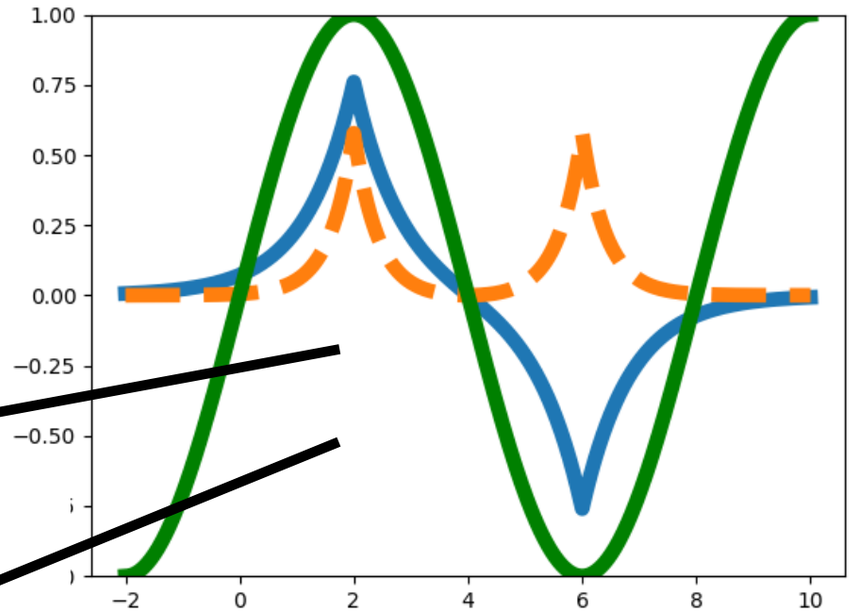

1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
0
5
10
15
20

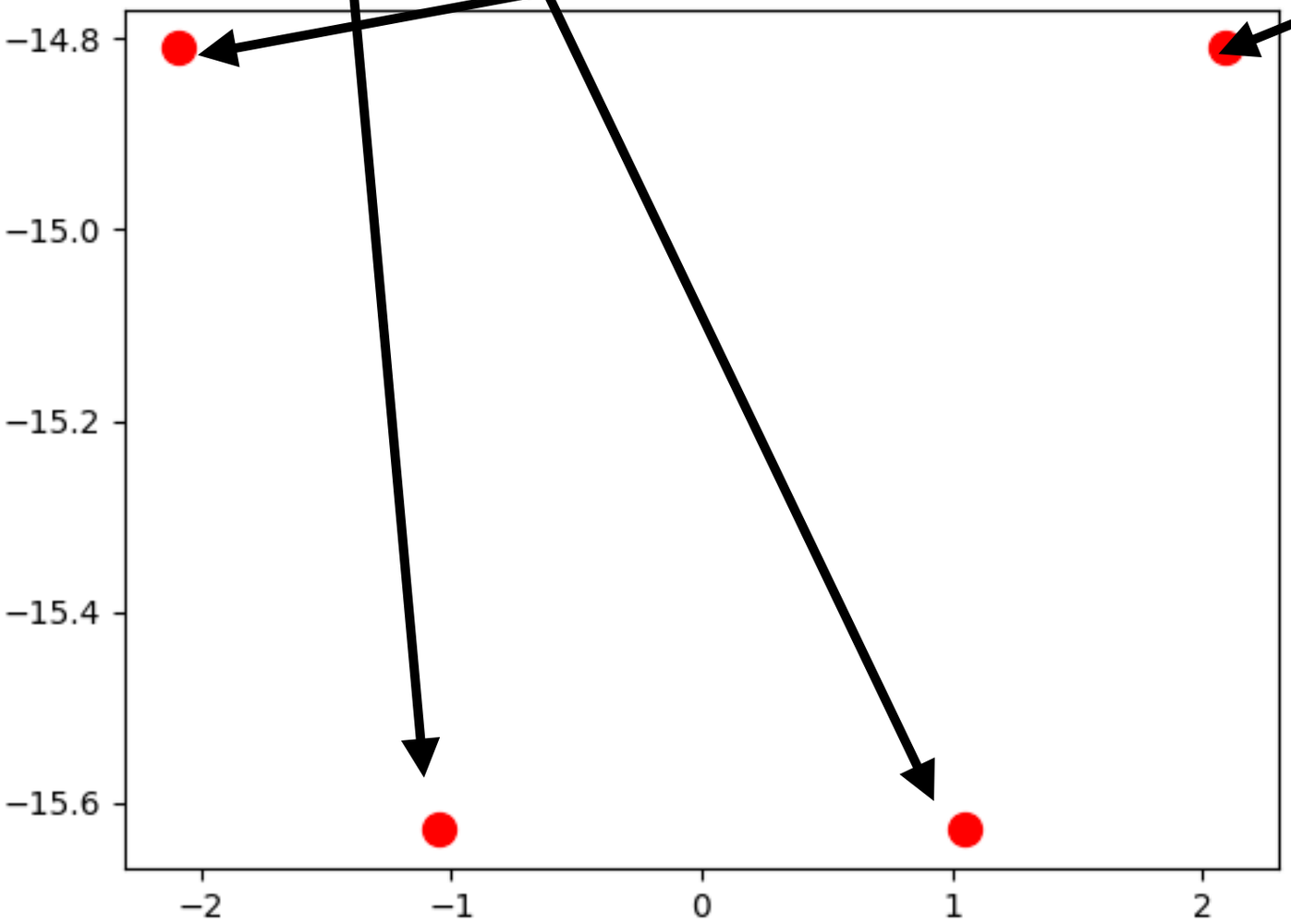

1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
0
5
10
15
20

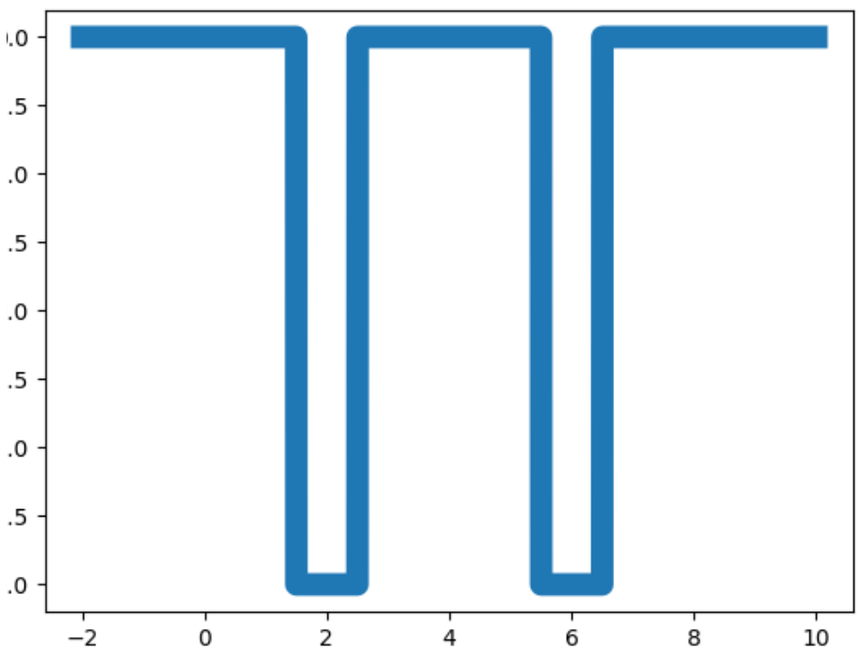

1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
0
5
10
15
20

Bloch Functions

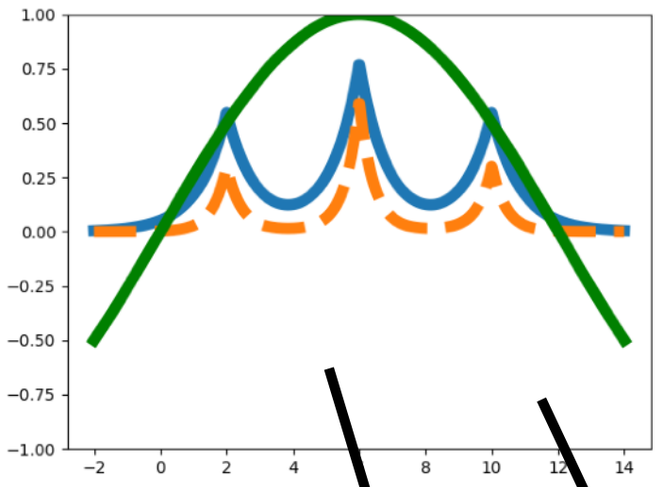


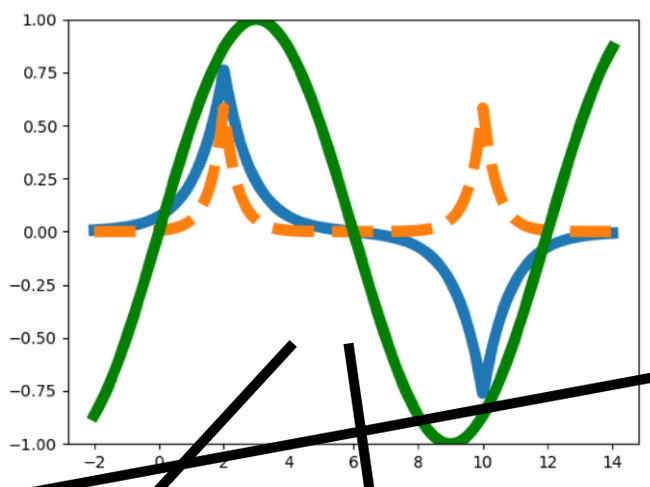


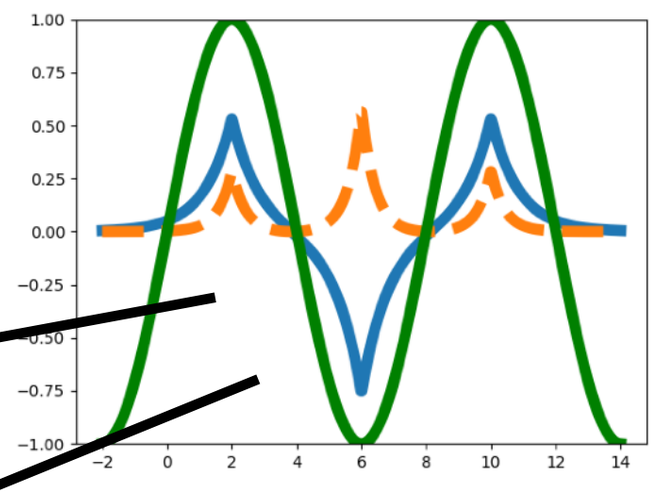


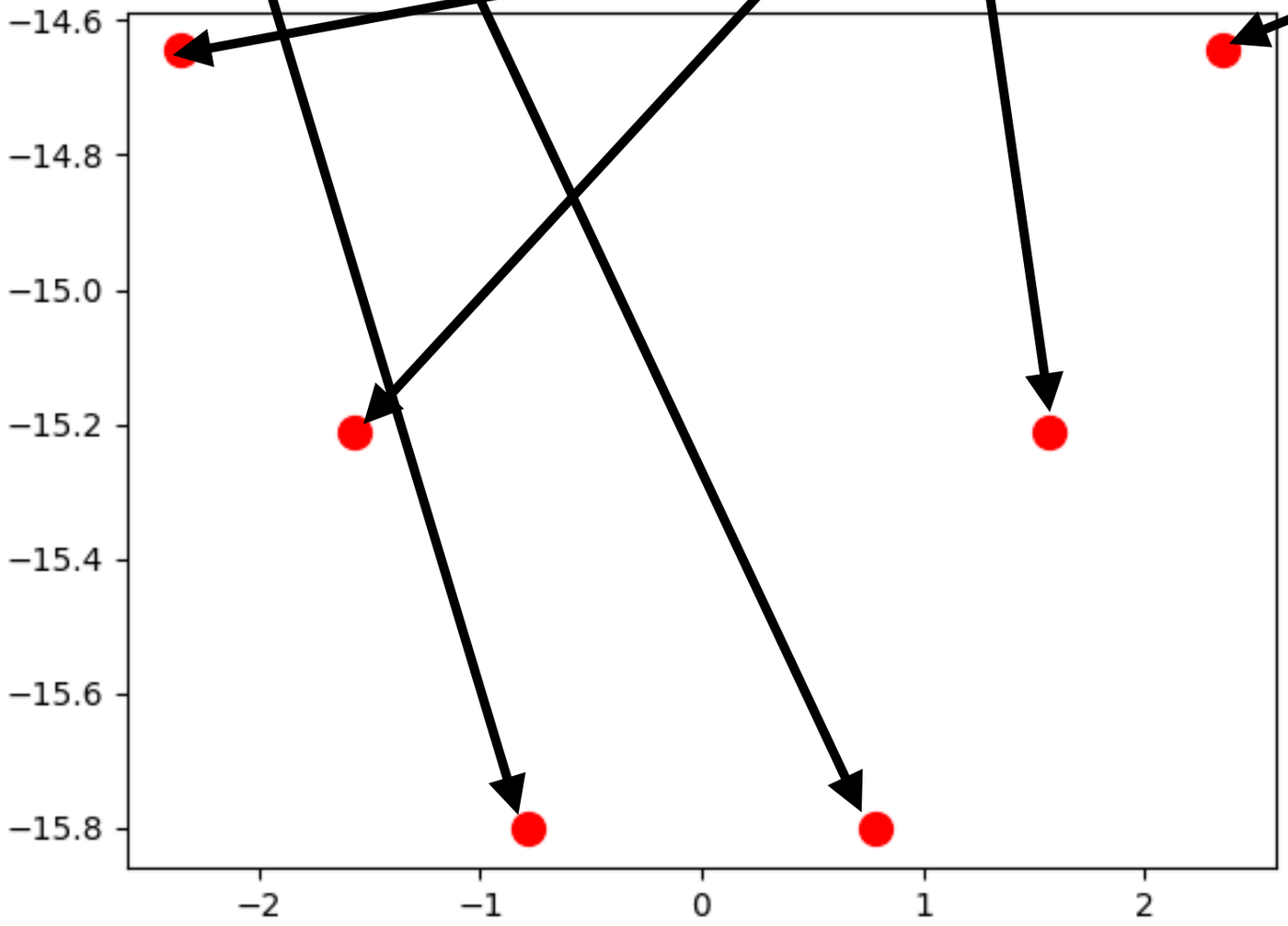


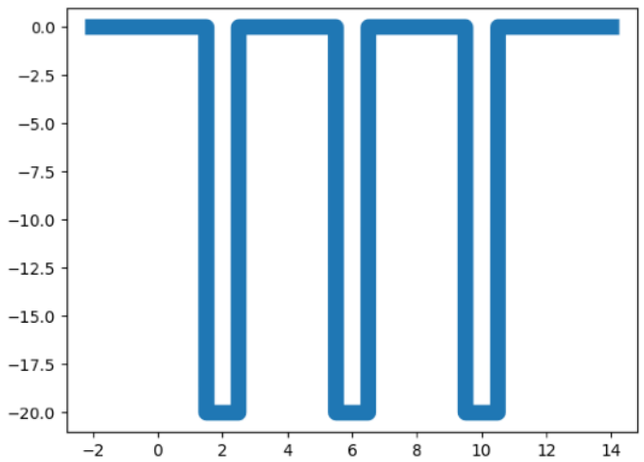
Bloch Functions



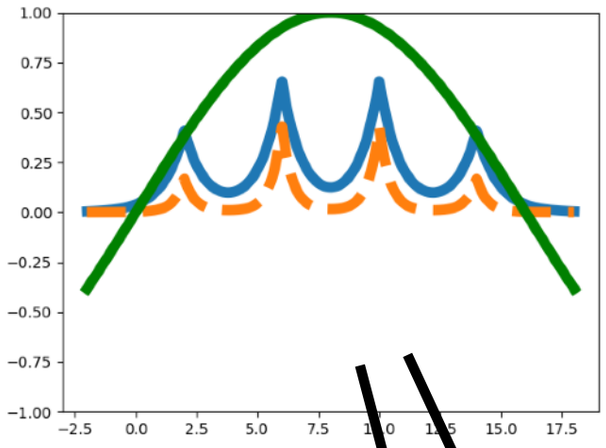


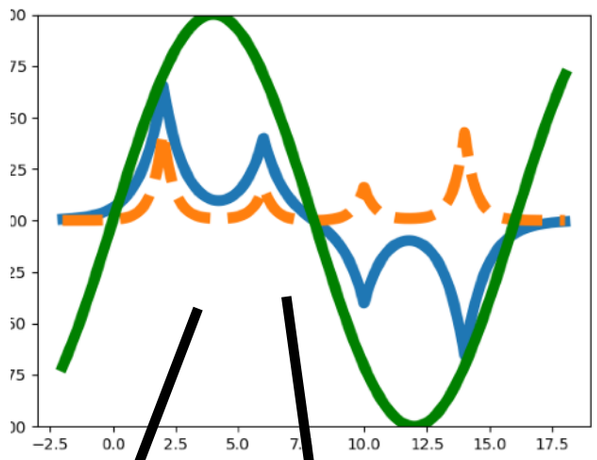


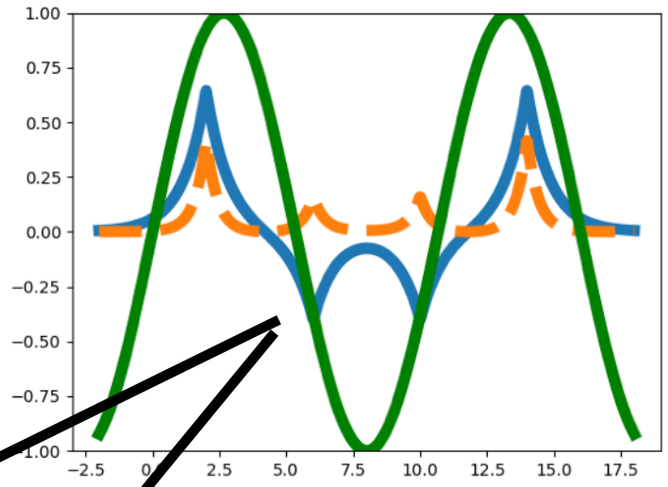


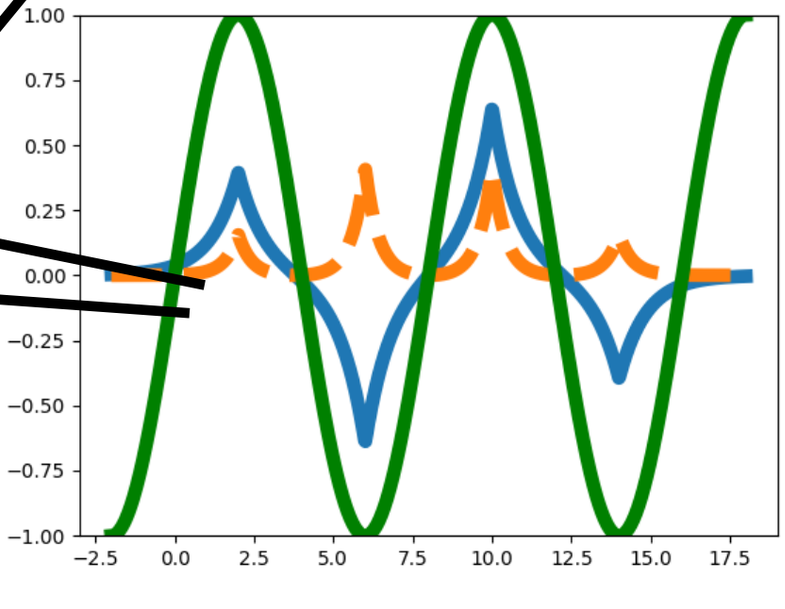


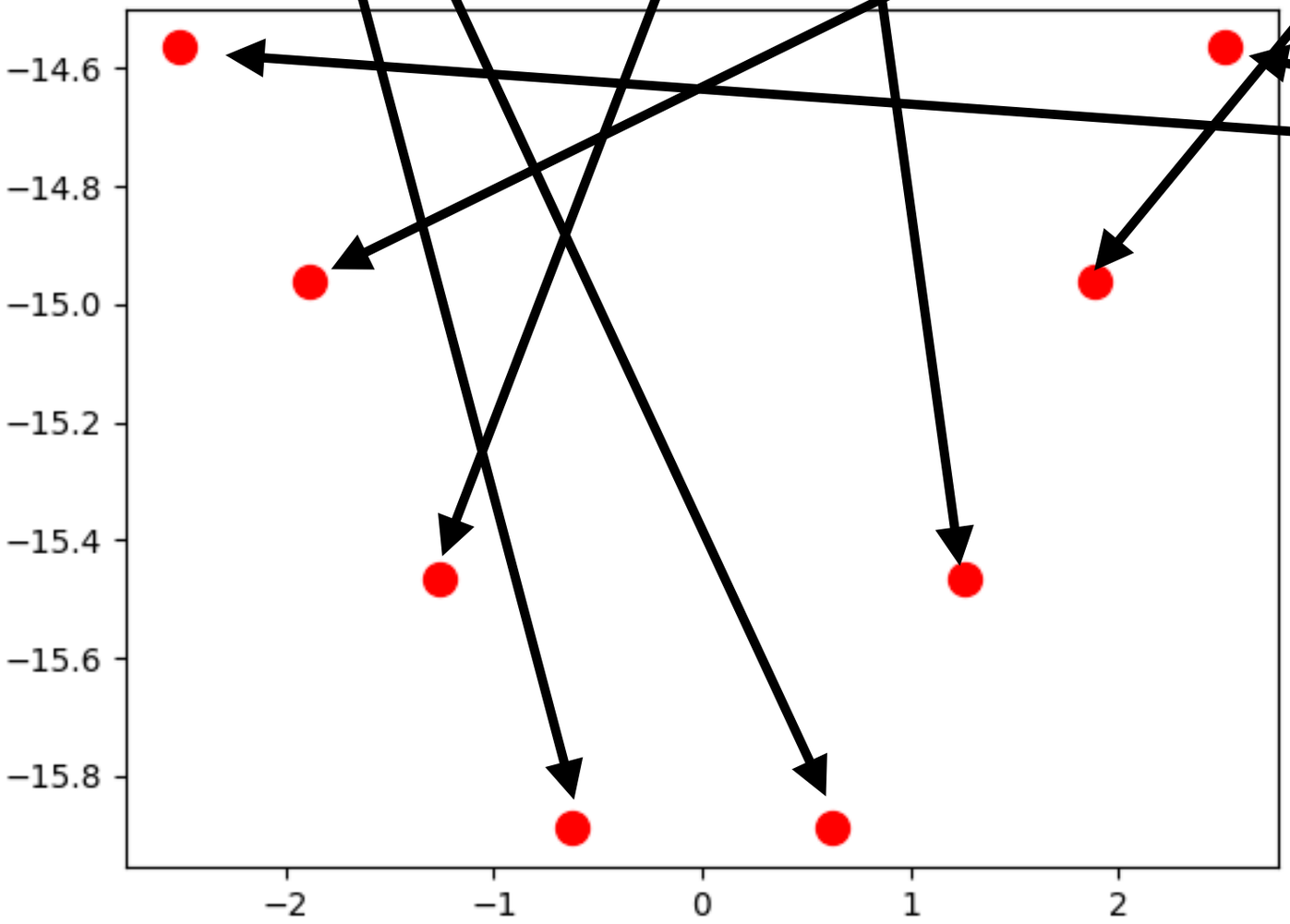
Bloch Functions

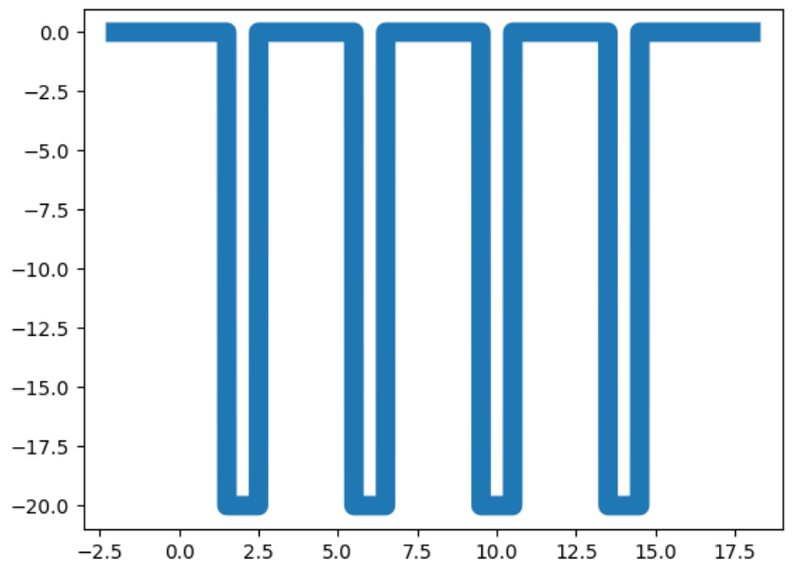




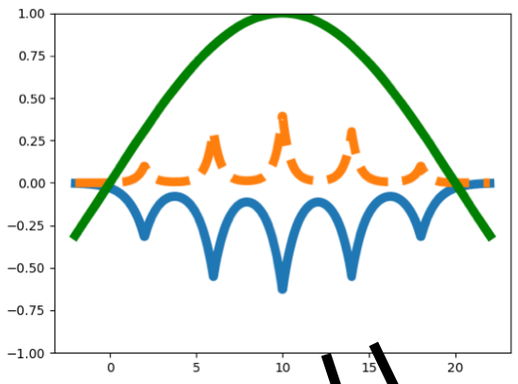


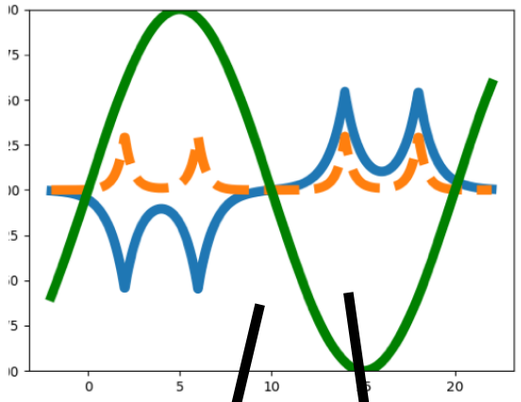


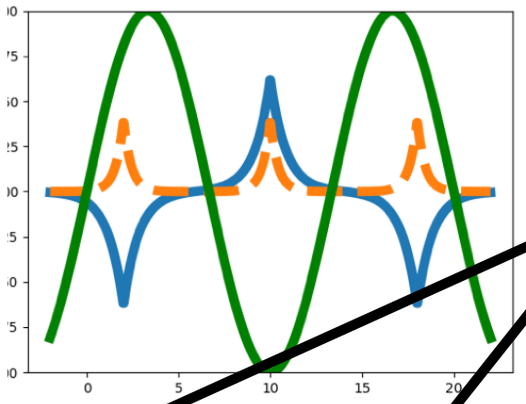


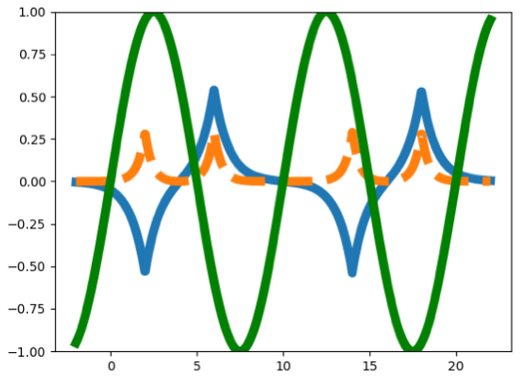


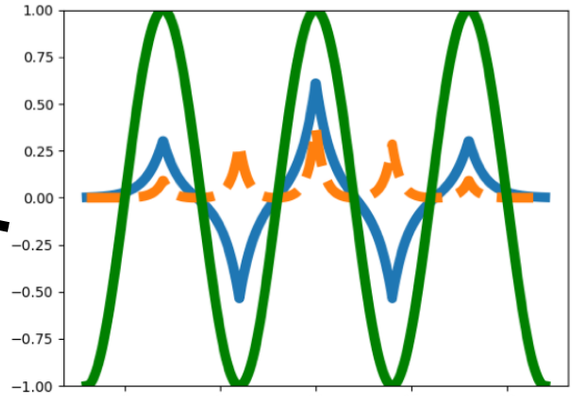
Bloch Functions

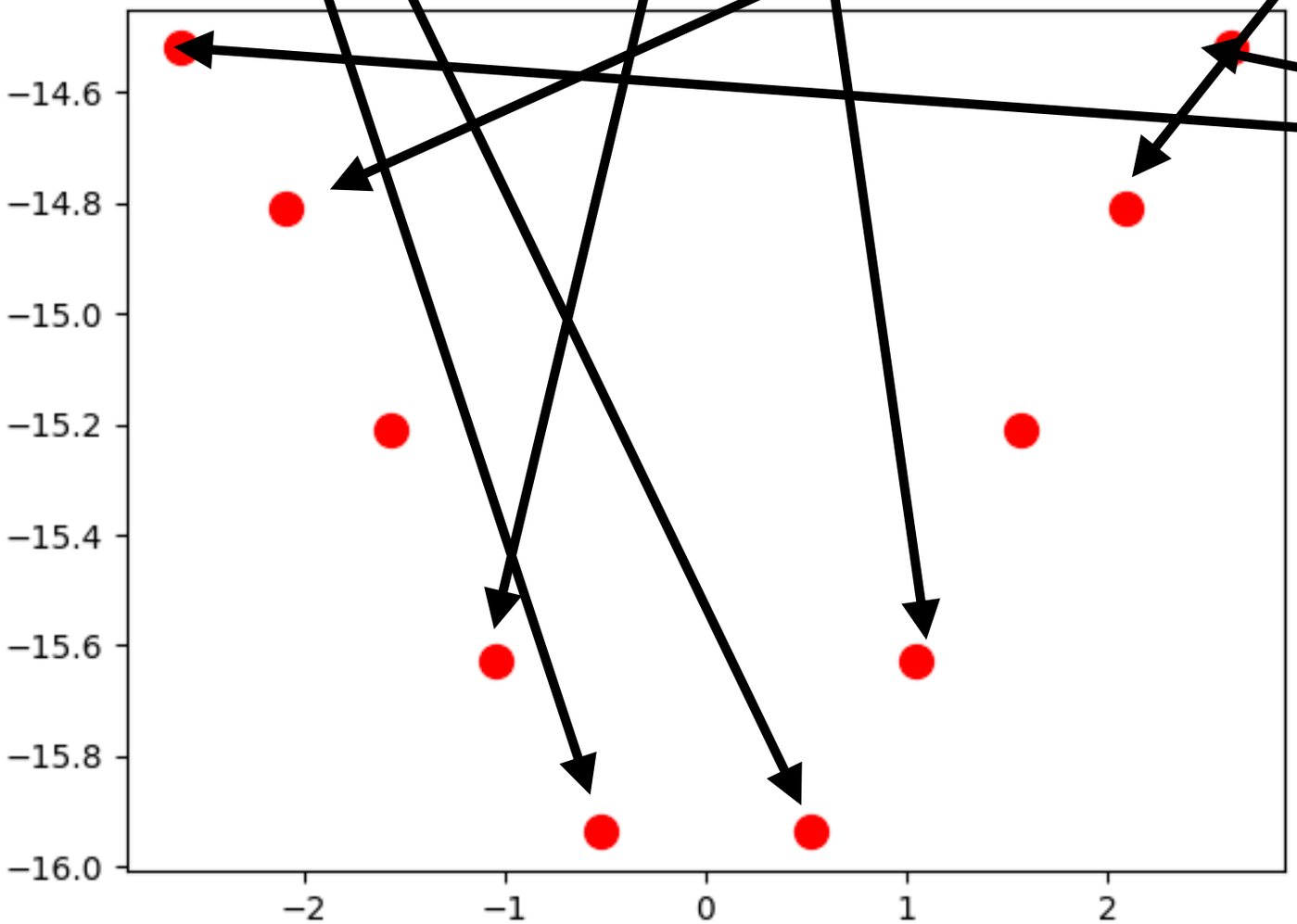


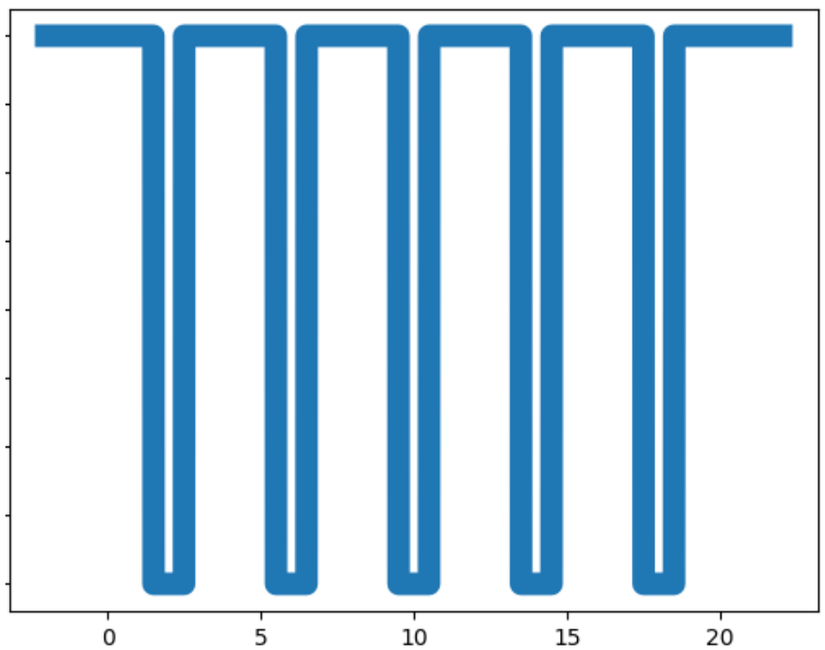




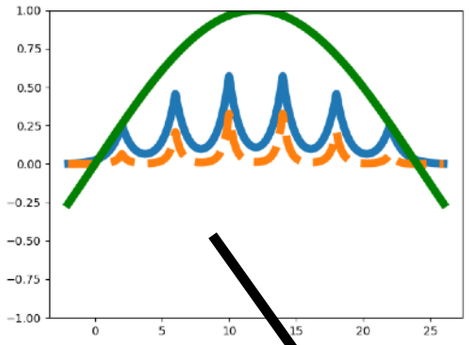


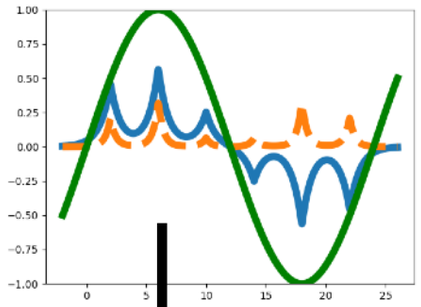


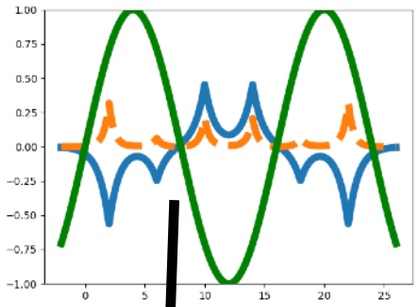


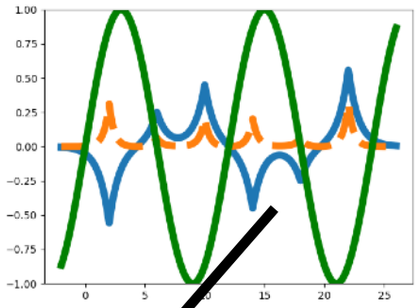


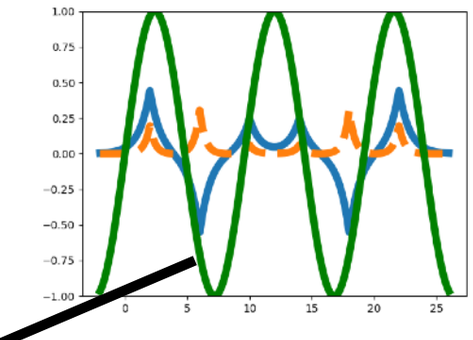
Bloch Functions

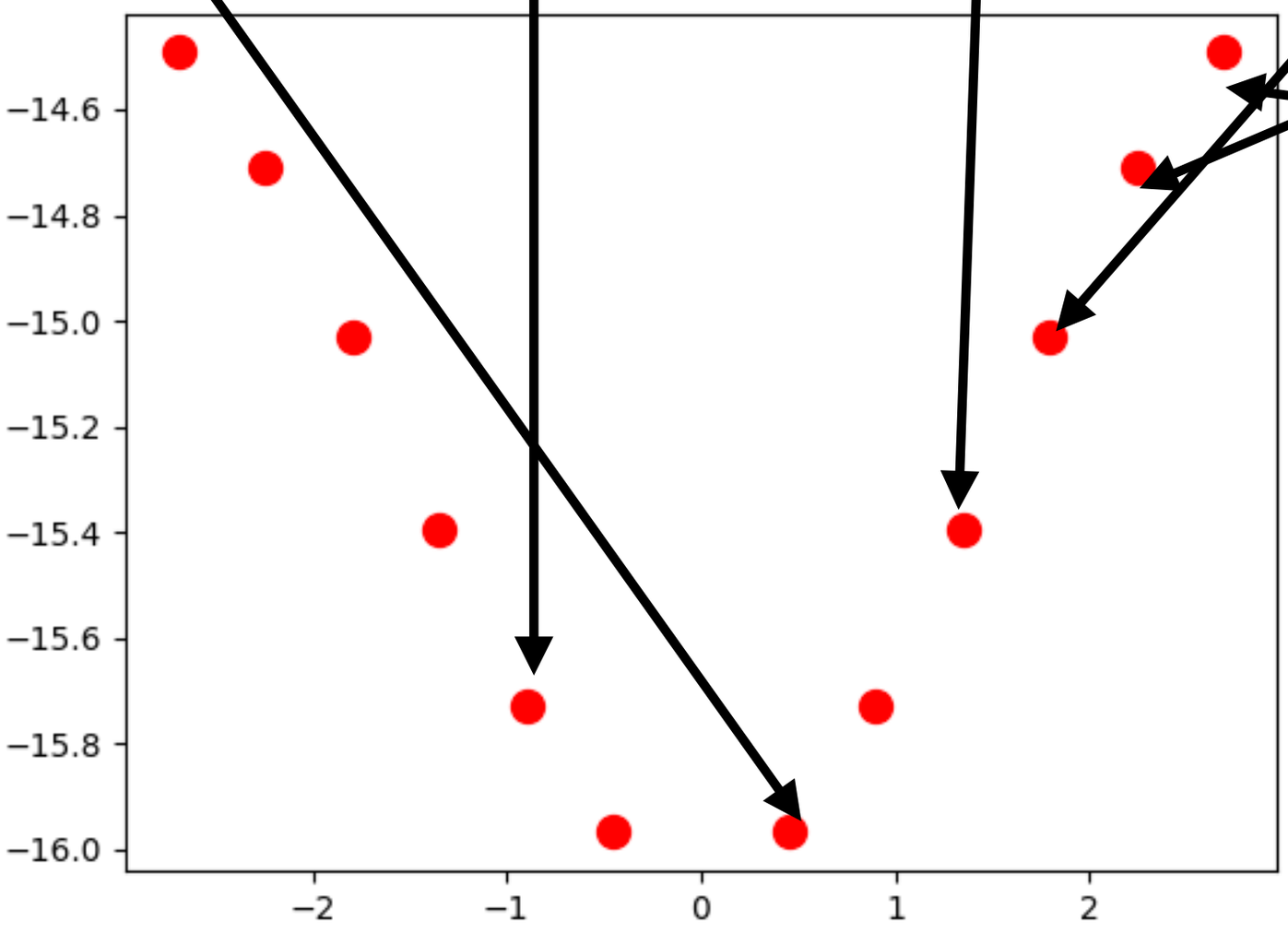


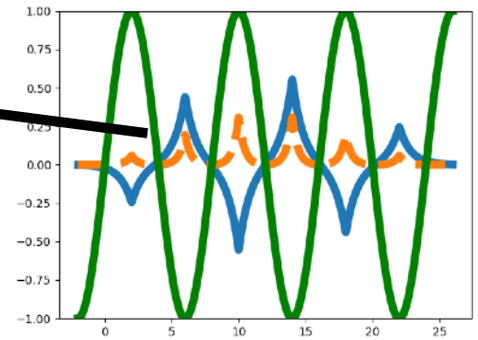


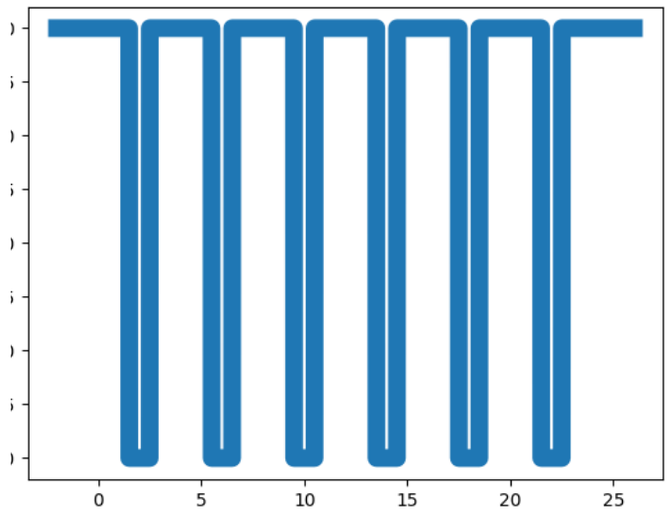




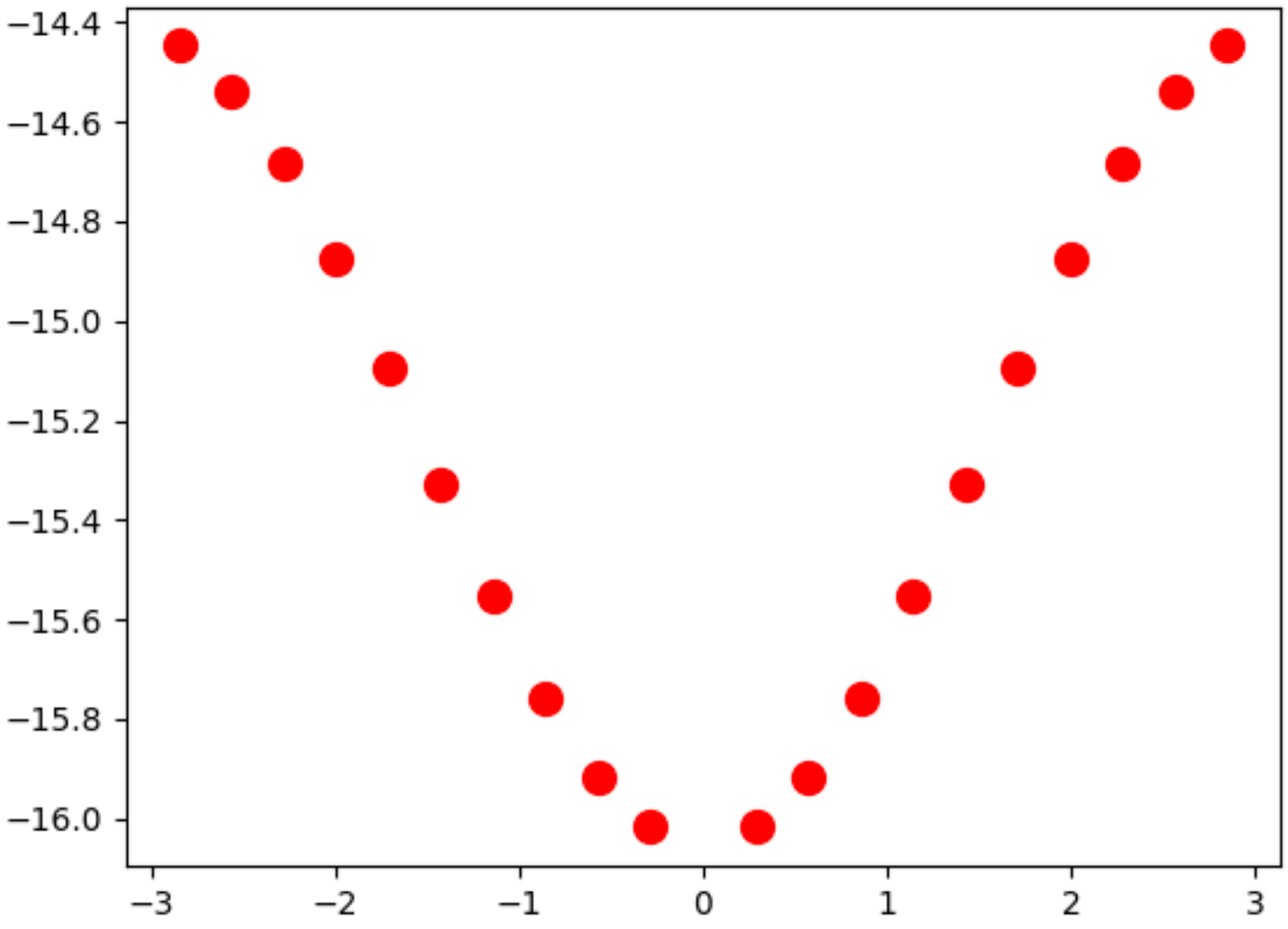








Bloch Functions



Important Points

$$\Psi(x) = e^{ikx} u(x)$$

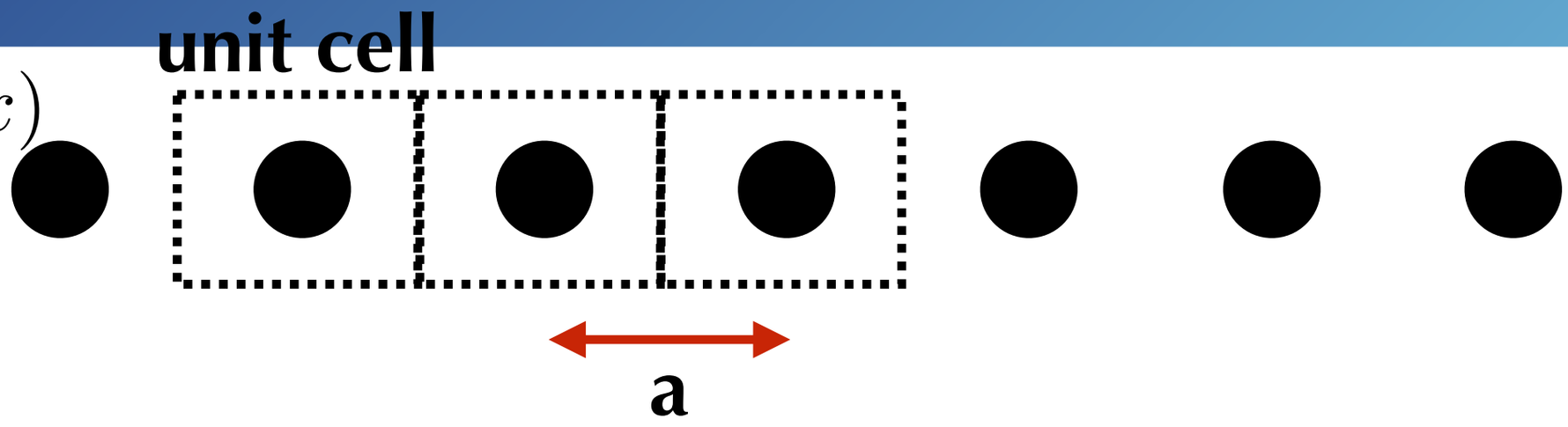
No longer need to loop over the entire atomic configuration

There is a k value (vector later) corresponding to every wave function.

For every k value (vector) there is an eigenvalue problem to solve.

Solving every eigenvalue problem on a grid of k values yields the band structure.

$$\Psi(x) = e^{ikx}u(x)$$



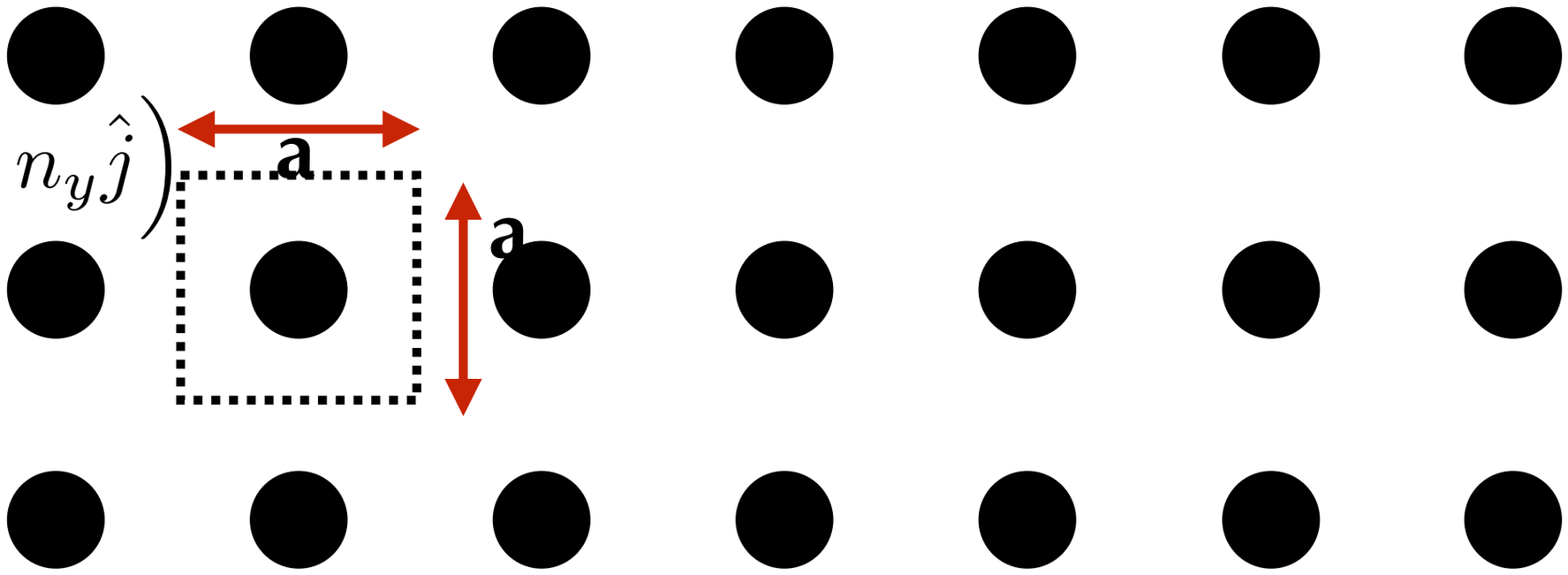
$$k = \frac{2\pi m}{Na}$$

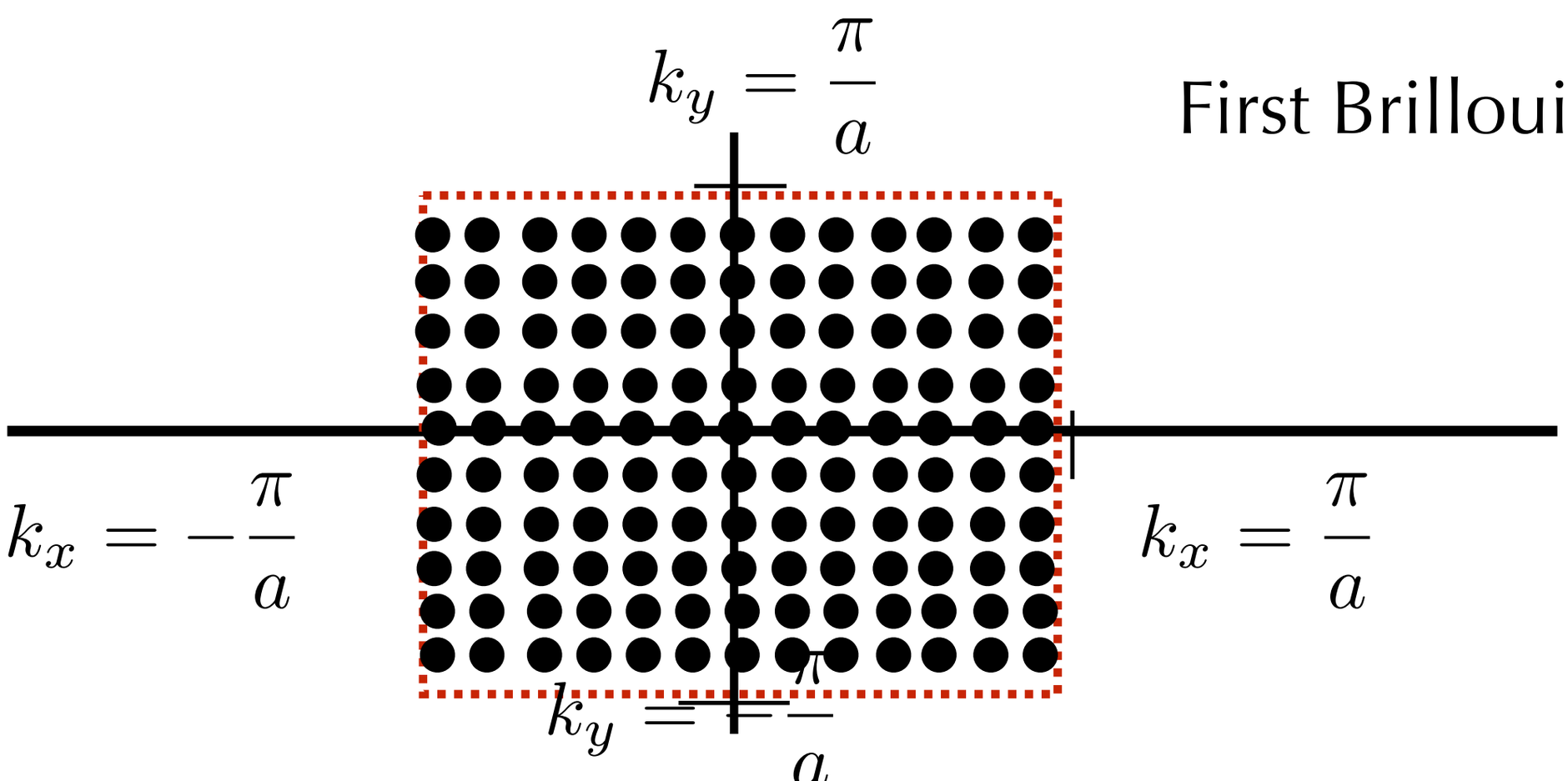
A repeating atomic configuration in real space leads to a solution that repeats in k-space.

A repeating atomic configuration in real space leads to a solution that repeats in k-space.

$$\Psi(x) = e^{i\mathbf{k}\cdot\mathbf{r}}$$

$$\mathbf{k} = \frac{2\pi}{L}\left(n_x\hat{i} + n_y\hat{j}\right)$$

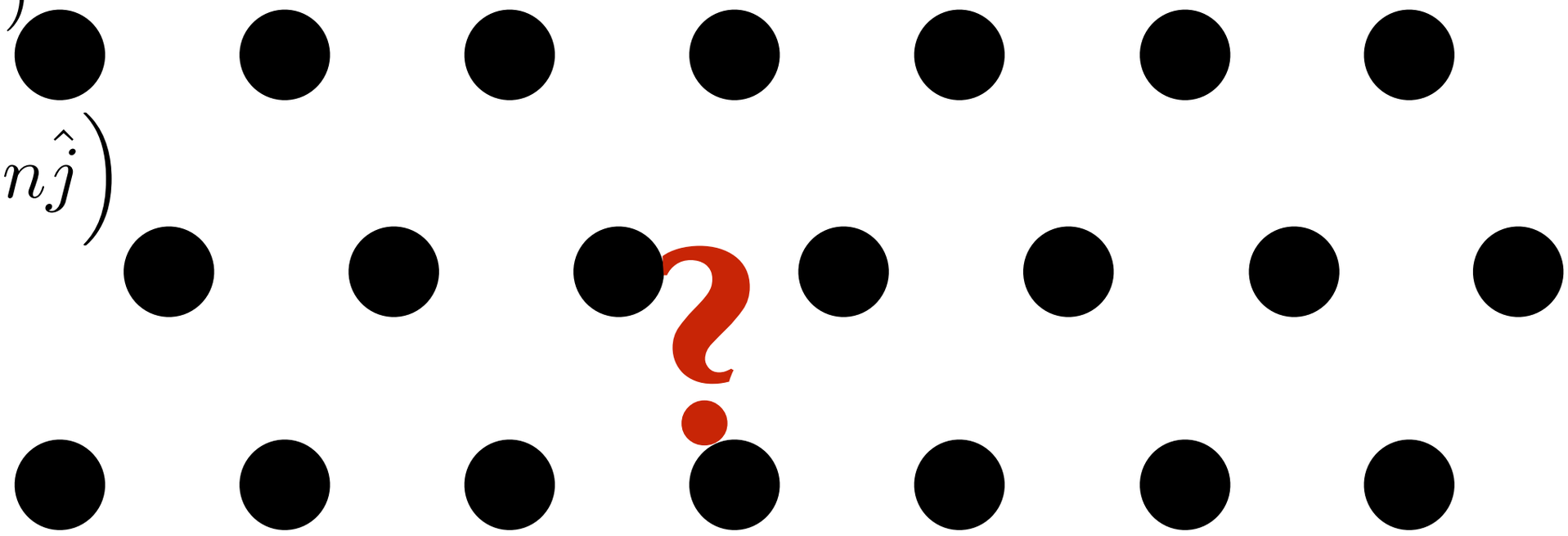


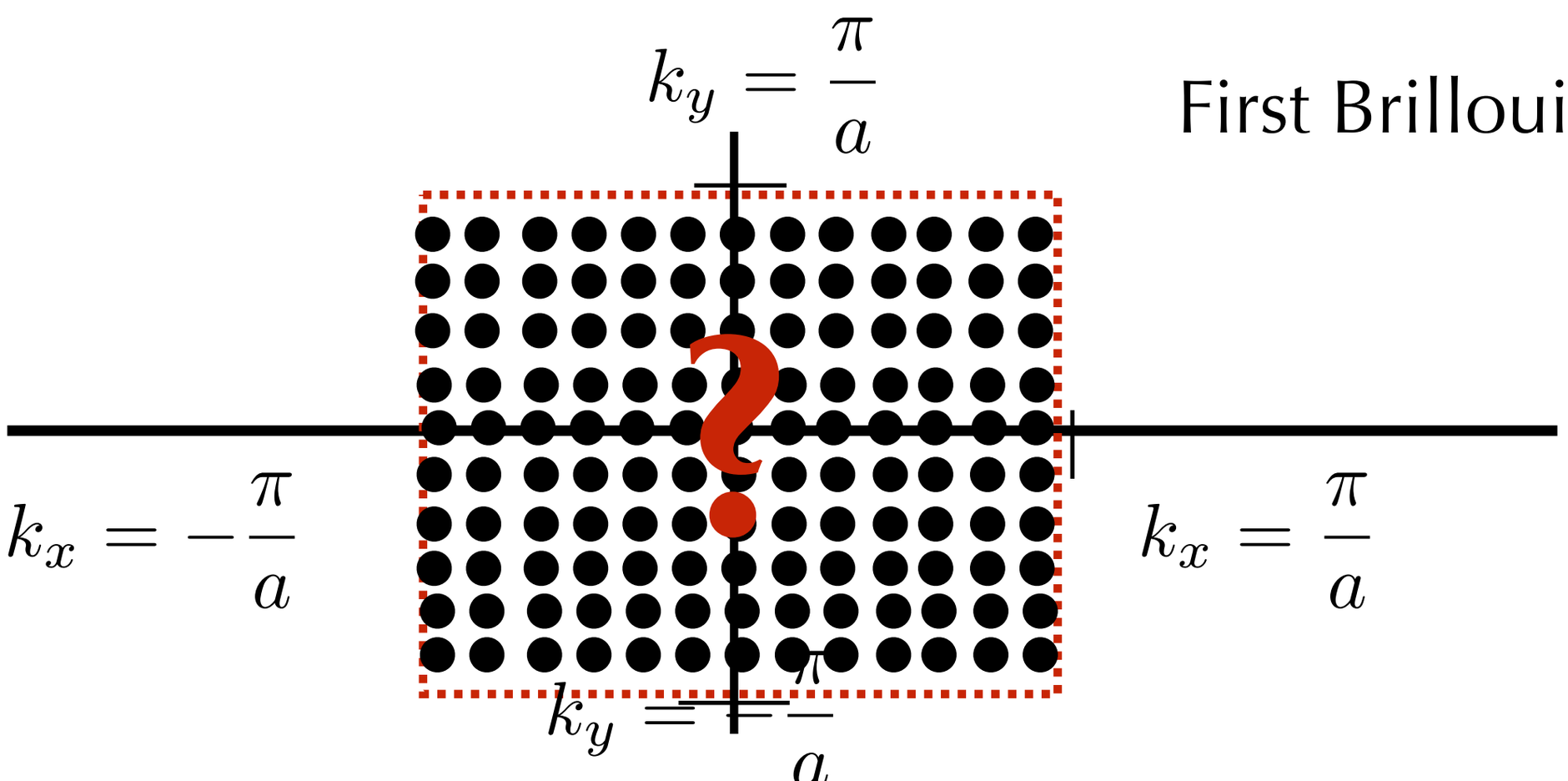


A repeating atomic configuration in real space leads to a solution that repeats in k-space.

$$\Psi(x) = e^{i\mathbf{k}\cdot\mathbf{r}}u(\mathbf{r})$$

$$\mathbf{k} = \frac{2\pi}{Na}\left(n\hat{i} + n\hat{j}\right)$$





First Brillouin Zone