Brillouin zone of two dimensional rectangle lattice

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Here we discuss the Brillouin zone for the two dimensional (2D)rectangle lattice using two problems of Kittel ISSP (8-th edition).

Chapter 9
1, 2
Kittel ISSP 8-th edition

1. Brillouin zones of rectangular lattice

Make a plot of the first two Brillouin zones of a primitive rectangular lattice with axes $a,\ b = 3a$ (Kittel ISSP 8-edition, 9-1)

((**Solution**))

The primitive lattice vector:

$$\boldsymbol{a}_1 = a\boldsymbol{e}_x , \qquad \boldsymbol{a}_2 = 3a\boldsymbol{e}_y$$

The reciprocal lattice vector:

$$\boldsymbol{b}_1 = \frac{2\pi}{a}\boldsymbol{e}_x , \boldsymbol{b}_2 = \frac{2\pi}{3a}\boldsymbol{e}_y$$

where

$$\boldsymbol{a}_1 \cdot \boldsymbol{b}_1 = 2\pi , \quad \boldsymbol{a}_2 \cdot \boldsymbol{b}_2 = 2\pi , \quad \boldsymbol{a}_1 \cdot \boldsymbol{b}_2 = \boldsymbol{a}_2 \cdot \boldsymbol{b}_1 = 0$$

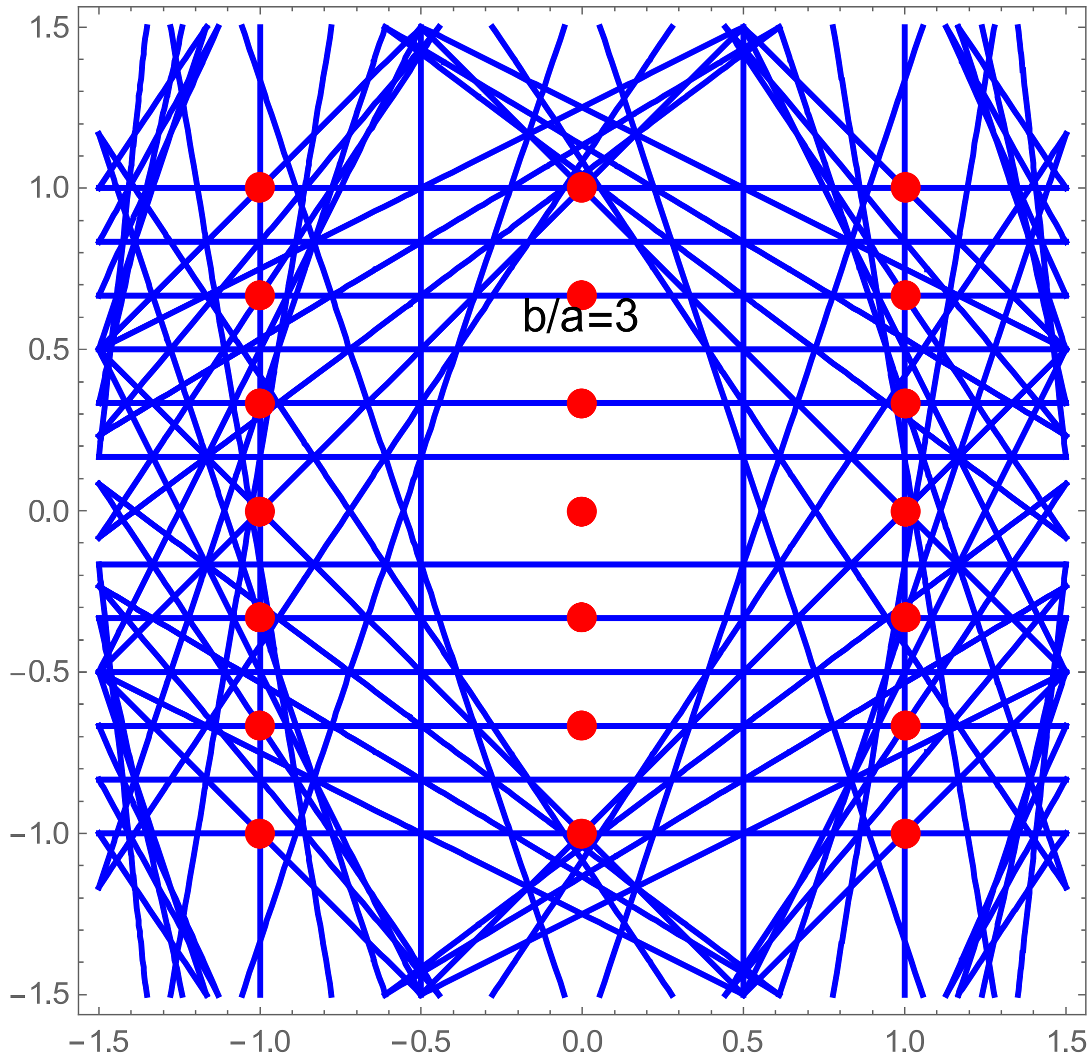

Fig. Brillouin zone for the 2D rectangular lattice with $b = 3a$, in the units of $(2\pi/a)$.

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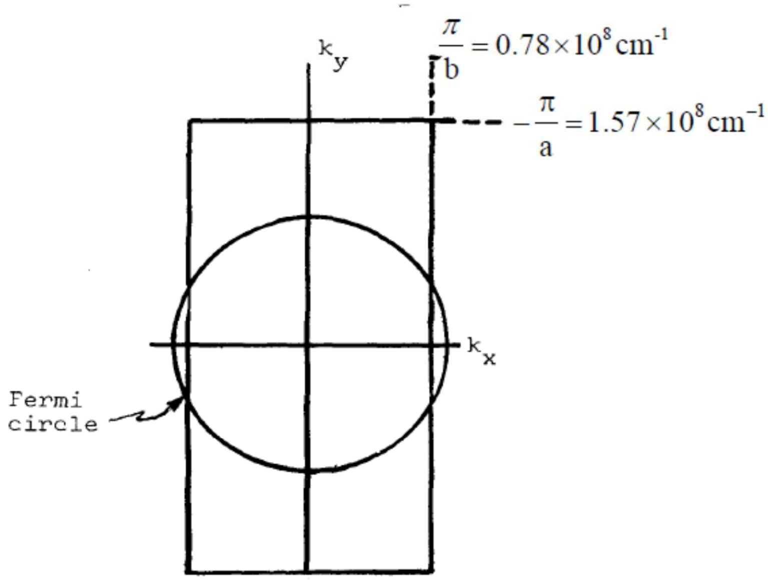
2. Brillouin zone, rectangle lattice (Kittel ISSP 9-2)

A 2D metal has one atom of valence one in a simple rectangular primitive cell $a = 2$ Å; $b = 4$ Å.
(a) Draw the first Brillouin zone. Give its dimensions, in cm^{-1}.
(b) Calculate the radius of the free electron Fermi sphere, in cm^{-1}.
(c) Draw this sphere to scale on a drawing of the first Brillouin zone. Make another sketch the first few periods of the free electron band in the periodic zone scheme, for both the first and second energy bands. Assume there is a small energy gap at the zone boundary

((**Solution by Kittel**))


$\frac{\pi}{b} = 0.78\times10^8\,cm^{-1}$
$-\frac{\pi}{a} = 1.57\times10^8\,cm^{-1}$
k_y
k_x
Fermi
circle

b.

$$N = 2 \times \frac{\pi k_F^2}{\left(2\pi / k\right)^2}$$

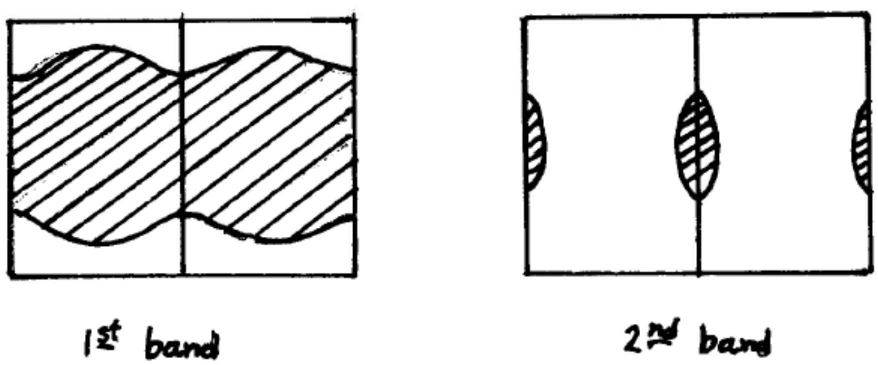
$$n = N/L^2 = k_F^2 / 2\pi$$

$$k_F = \sqrt{2\pi n}$$

$$n = \frac{1}{8} \times 10^{16} \mathrm{els/cm^2}$$

$$k_F = 0.89 \times 10^8 \mathrm{cm^{-1}}$$

c.



((**Solution**))
(a)

The primitive lattice vector:

$$\boldsymbol{a}_1 = a\boldsymbol{e}_x, \qquad \boldsymbol{a}_2 = b\boldsymbol{e}_y = 2a\boldsymbol{e}_y \qquad \text{with } a = 2\text{Å},\ b = 4\ \text{Å}.$$

The reciprocal lattice vector:

$$\boldsymbol{b}_1 = \frac{2\pi}{a}\boldsymbol{e}_x, \boldsymbol{b}_2 = \frac{2\pi}{2a}\boldsymbol{e}_y = \frac{\pi}{a}\boldsymbol{e}_y$$

where

$$\boldsymbol{a}_1 \cdot \boldsymbol{b}_1 = 2\pi, \quad \boldsymbol{a}_2 \cdot \boldsymbol{b}_2 = 2\pi, \quad \boldsymbol{a}_1 \cdot \boldsymbol{b}_2 = \boldsymbol{a}_2 \cdot \boldsymbol{b}_1 = 0$$

$$\frac{\pi}{a} = 1.57\ \text{Å}^{-1}. \qquad \frac{\pi}{b} = 0.785\ \text{Å}^{-1}.$$

(b) Fermi sphere

$$N = \frac{2A}{(2\pi)^2}\pi k_F{}^2, \qquad n = \frac{N}{A} = \frac{k_F{}^2}{2\pi} = \frac{N_0}{ab}$$

where there are N_0 electrons per unit cell ($a \times b$)

$$k_F = \sqrt{2\pi \frac{N_0}{ab}}$$

When $N_0 = 1$, $a = 2$ Å, $b = 2a$,

$$k_F = \frac{\sqrt{\pi}}{a} = k_F = 8.862 \times 10^7\ \text{cm}^{-1}.$$

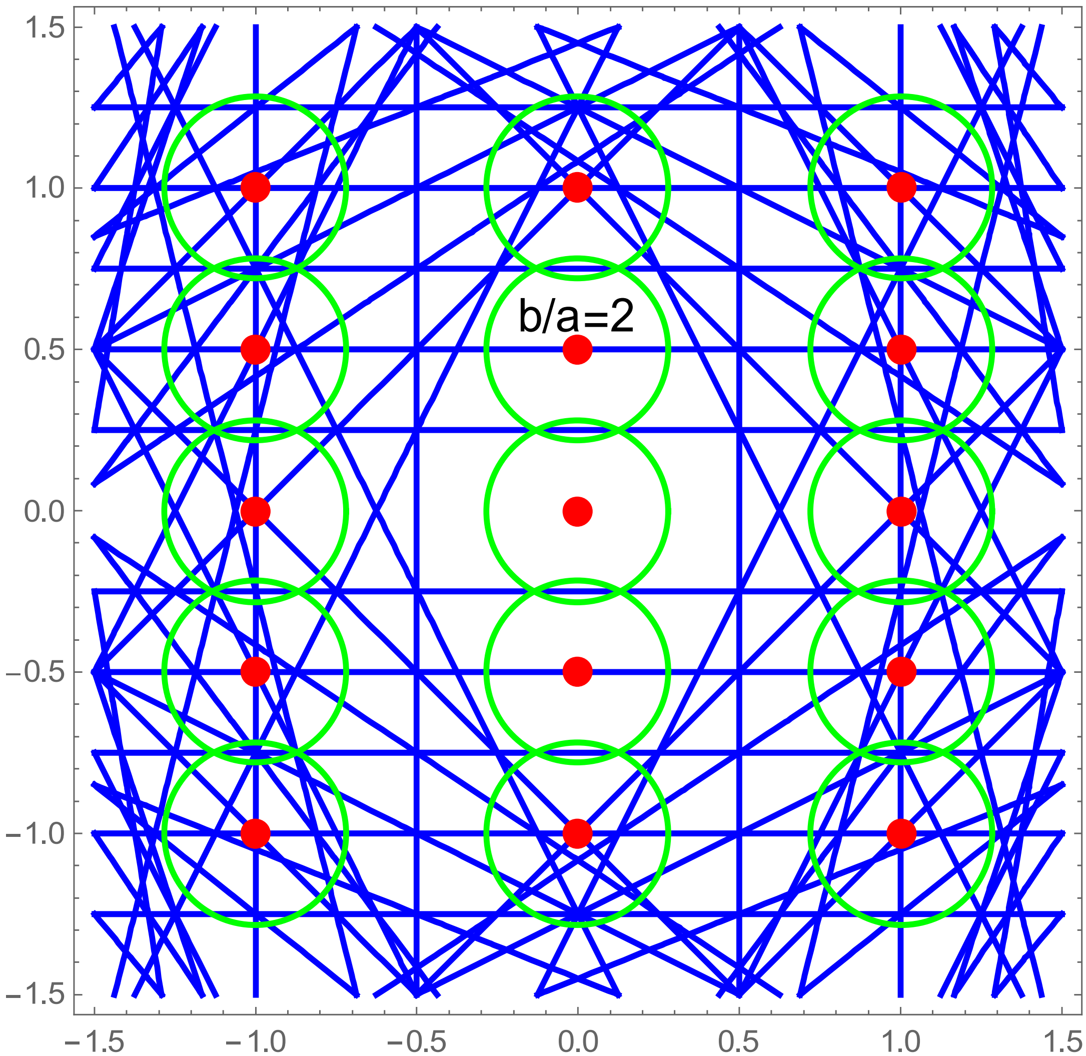


Fig. $b = 2a$. $N_0 = 1$. There is 1 electron per unit cell.

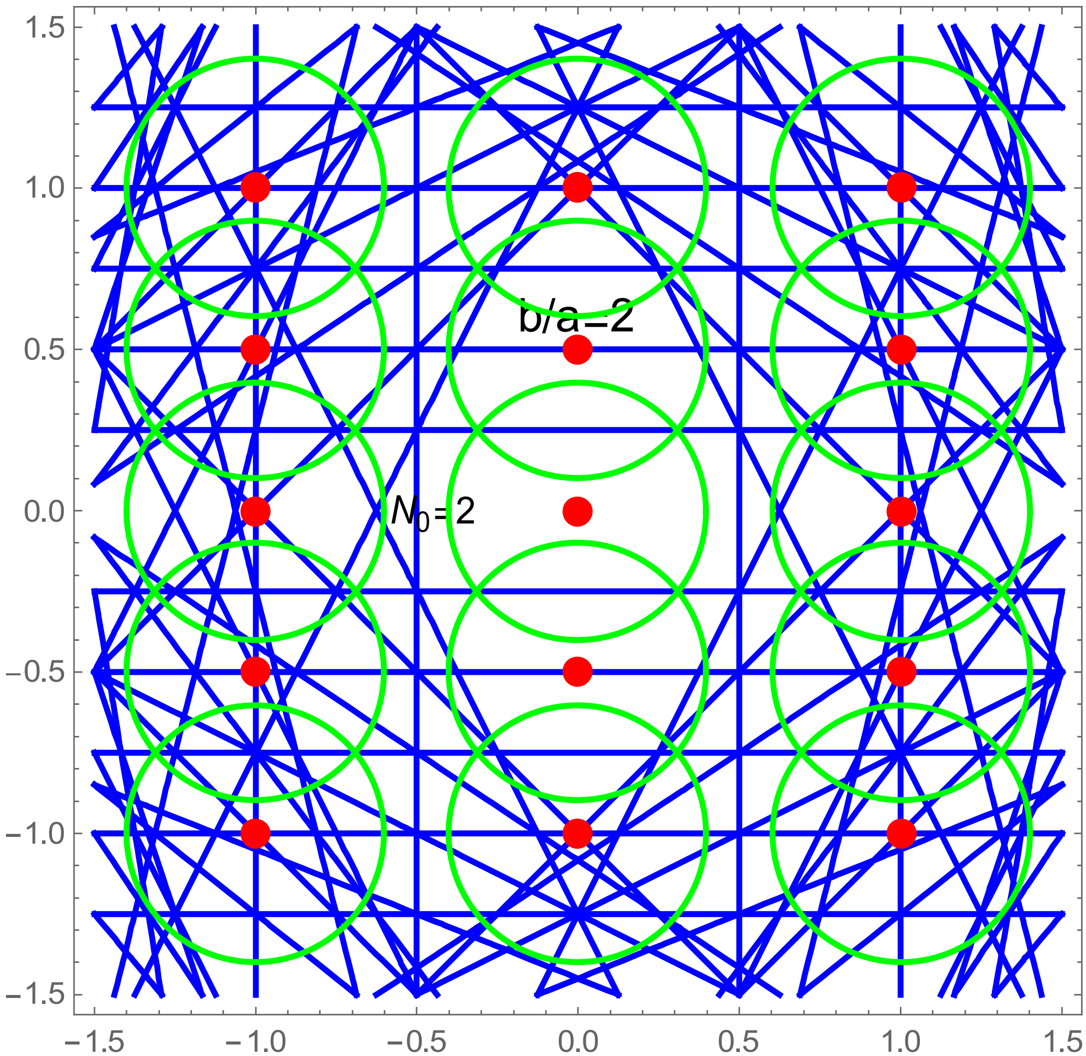


Fig. $b = 2a$. $N_0 = 2$. There are 2 electron per unit cell.

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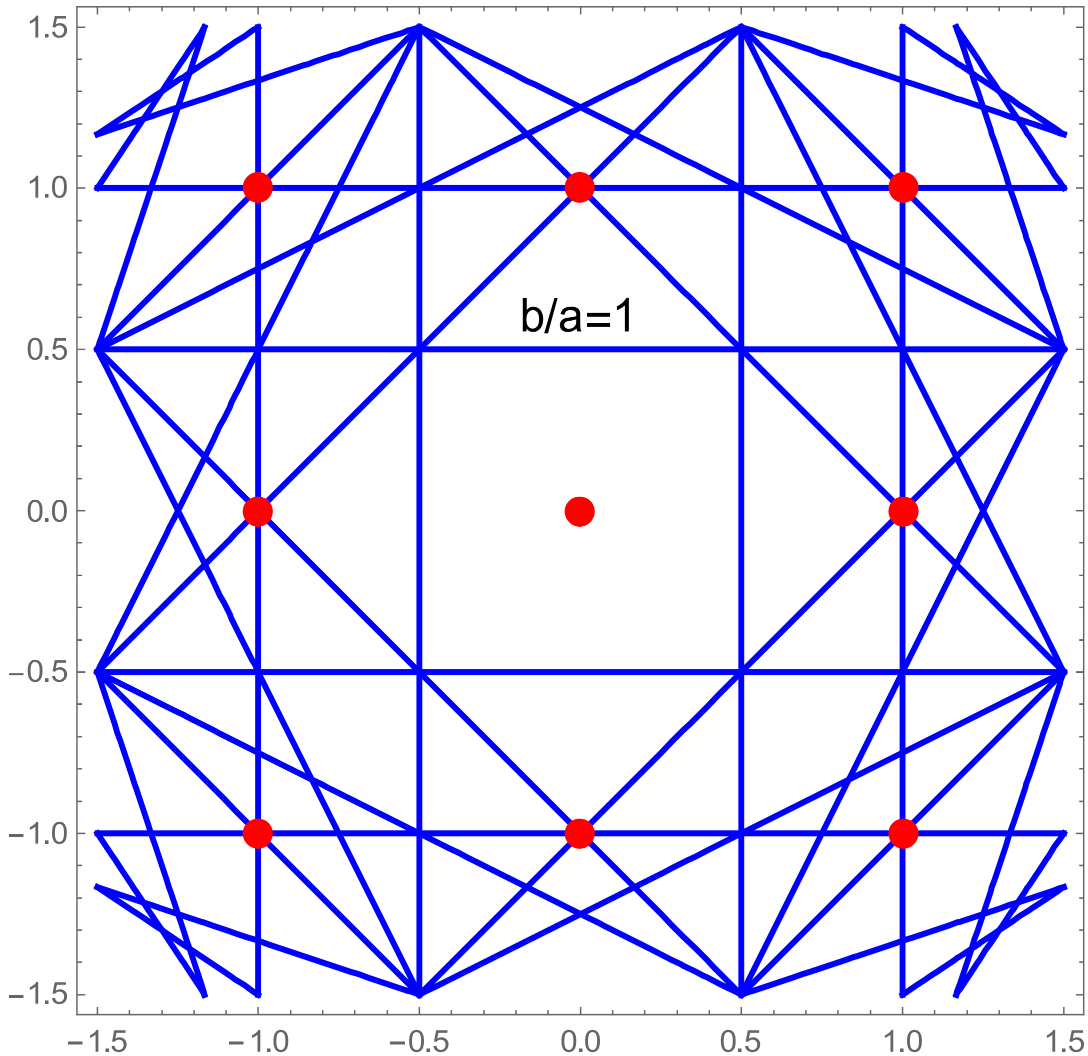
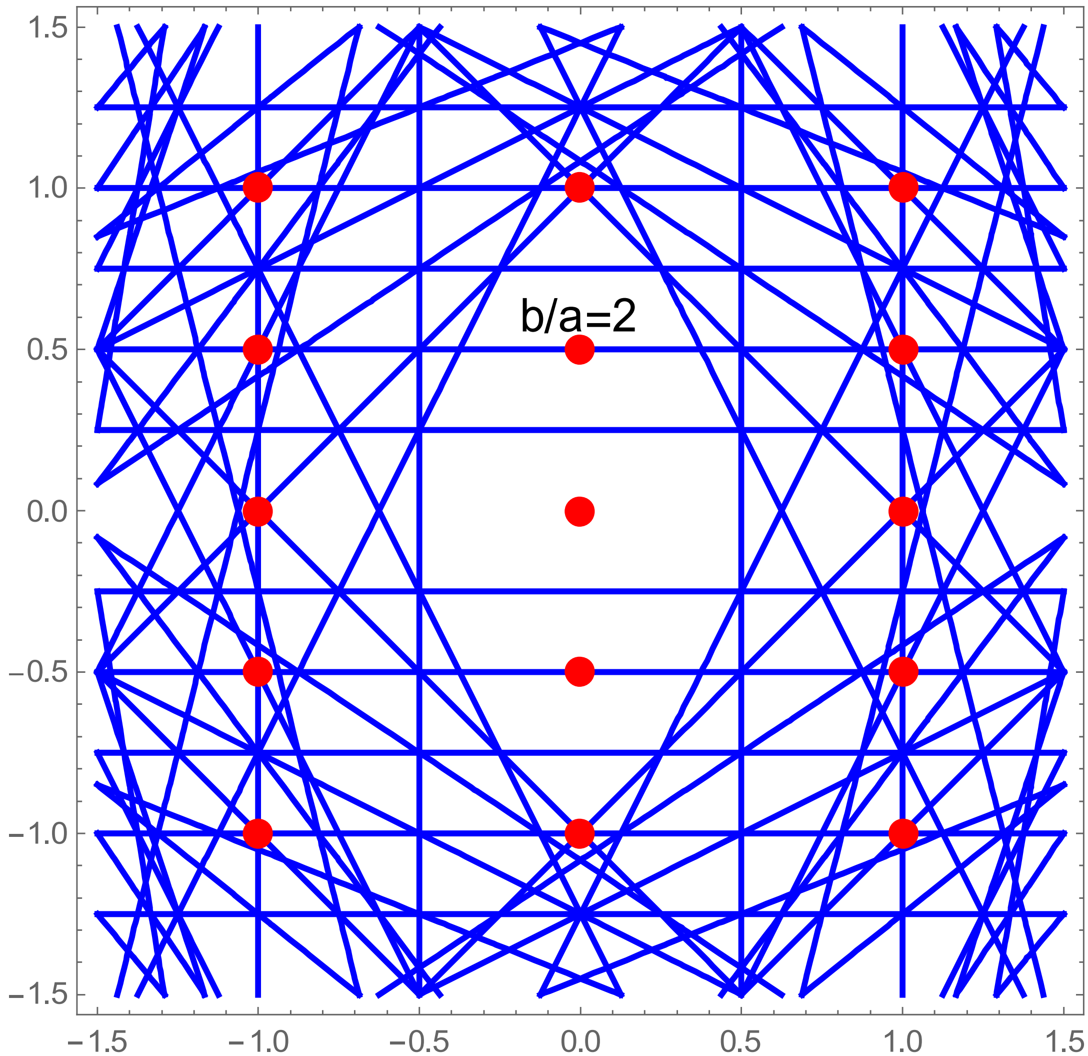
3. Brillouin zone of 2D rectangle lattice with lattice ($a \times b(= na)$ with n = 1, 2, 3, ……

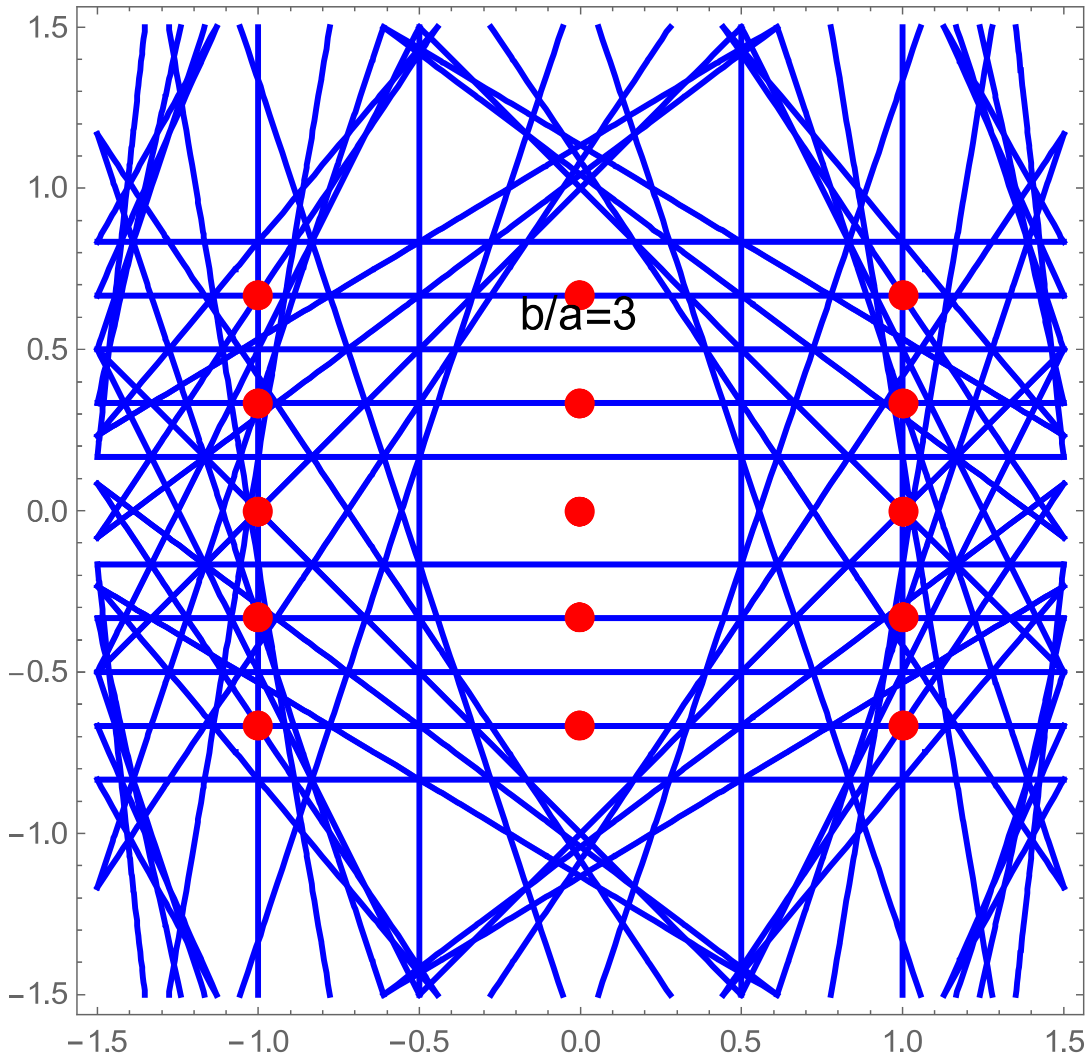
(1) 2D square lattice ($b = a$)



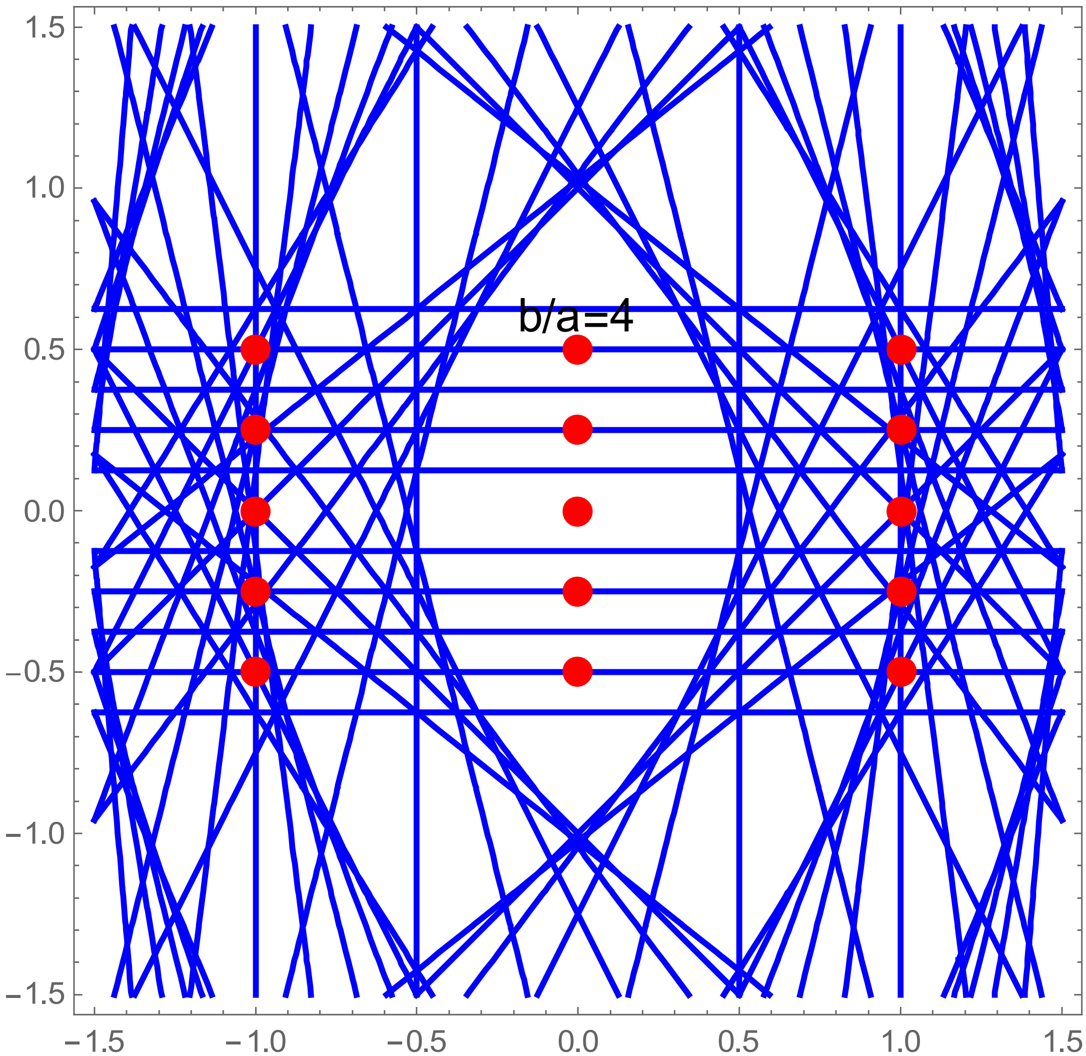
(b) 2D rectangle lattice ($b = 2a$)



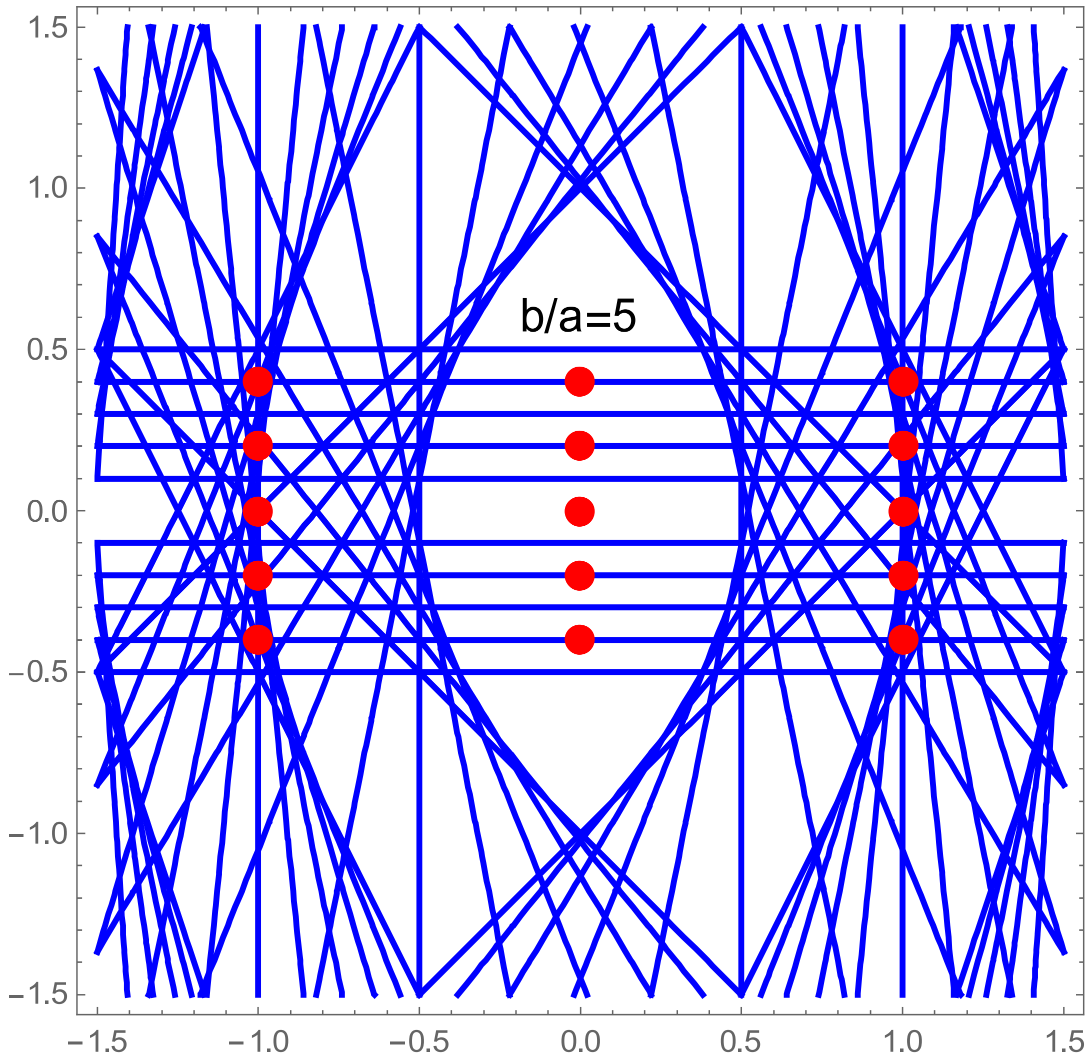
(c) 2D rectangle lattice ($b = 3a$)



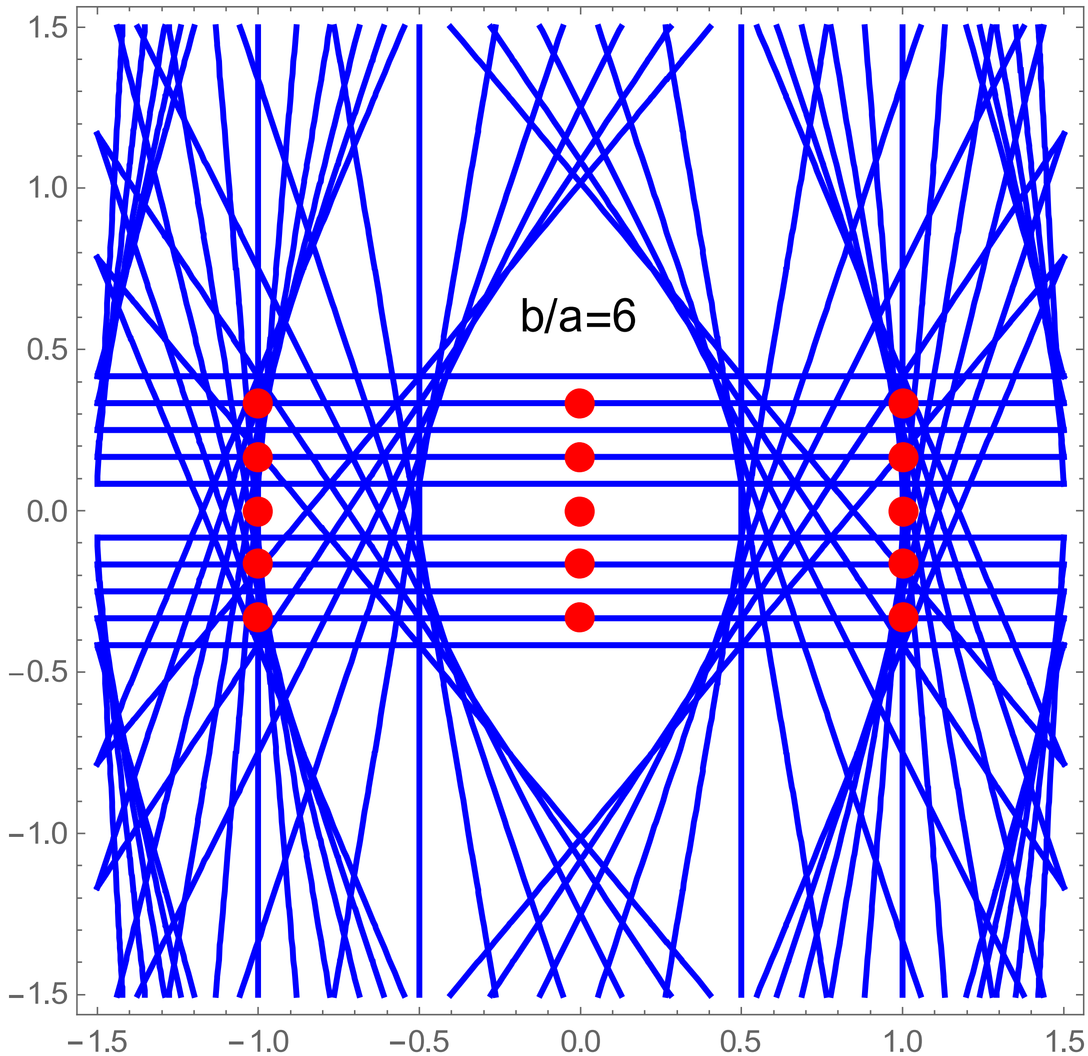
(d) 2D rectangle ($b = 4a$)

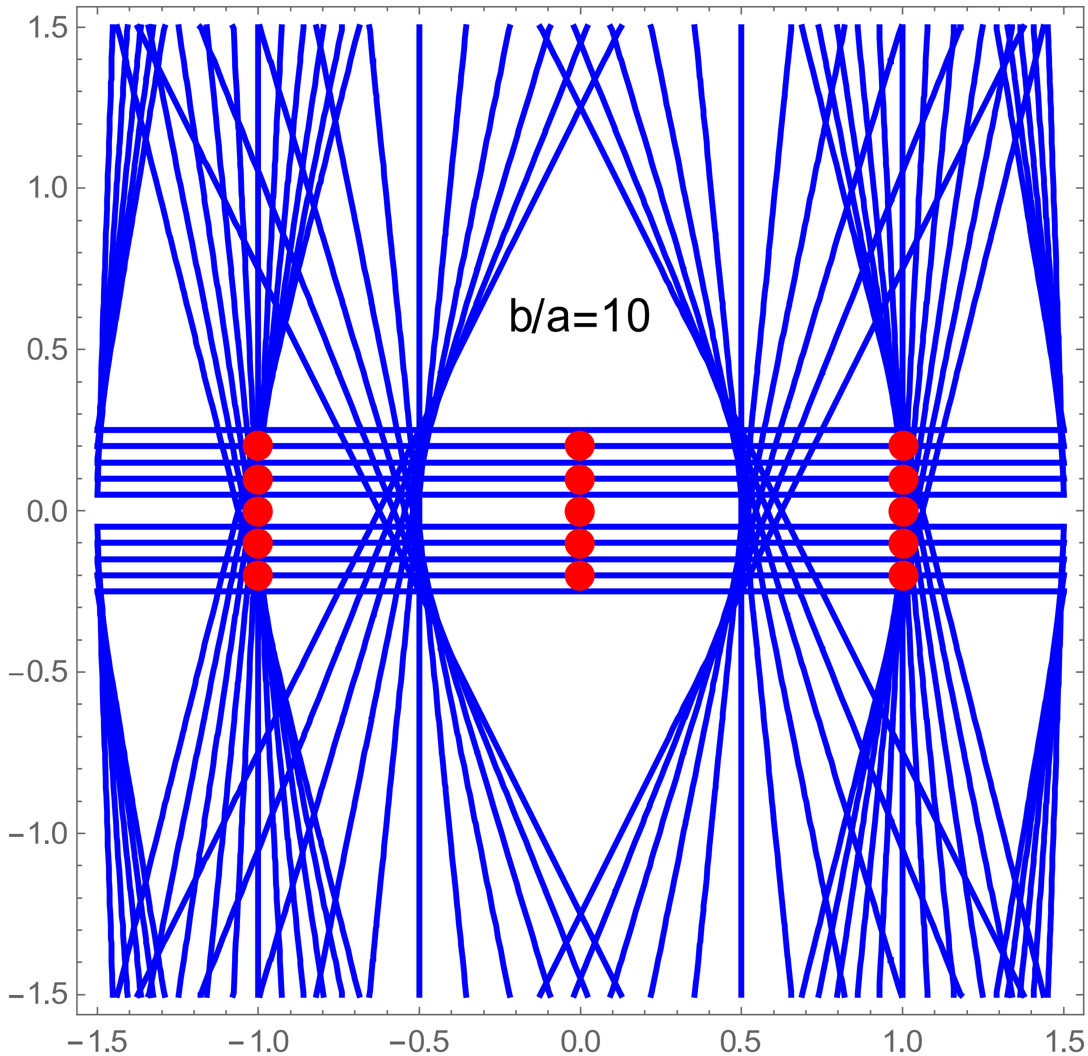


(e) 2D rectangle lattice ($b = 6a$)



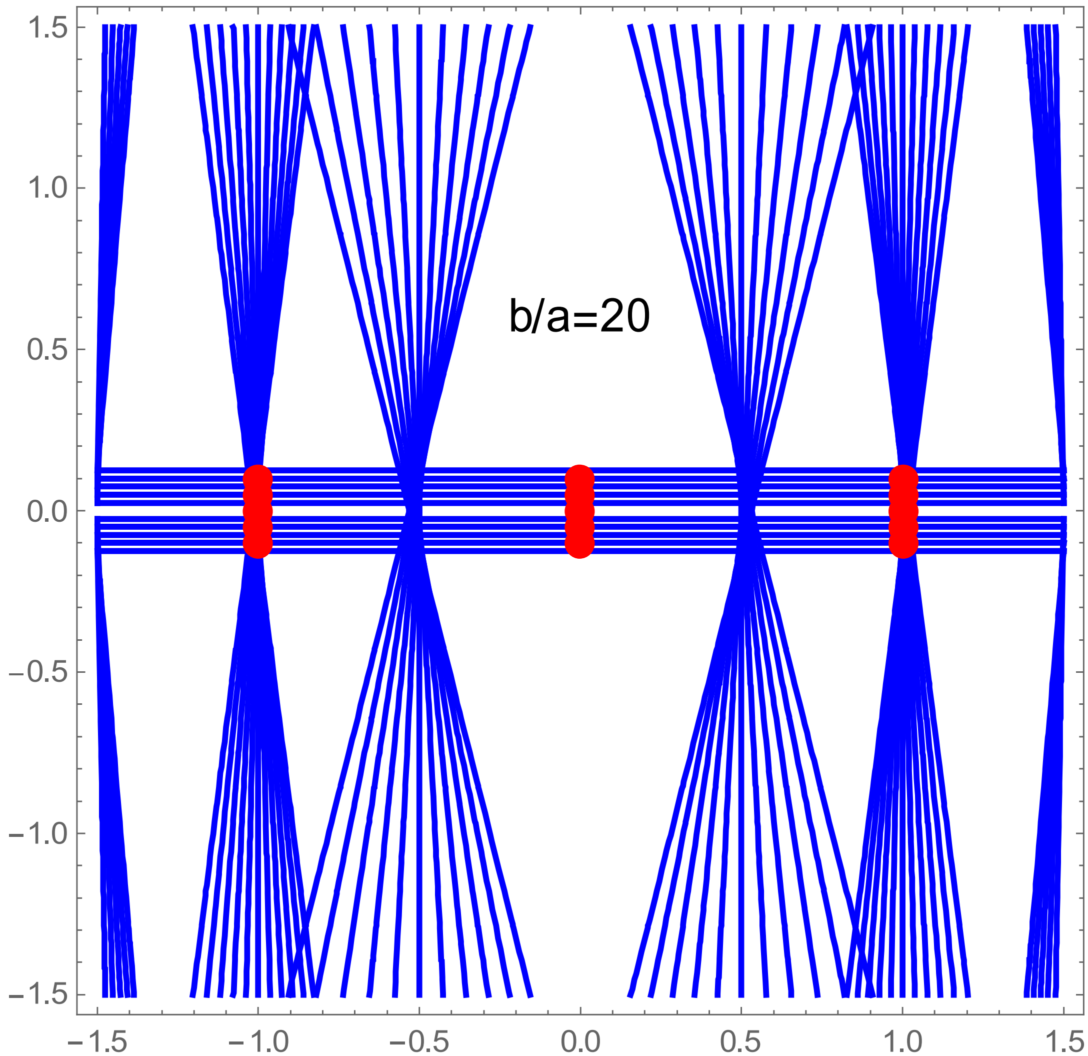
b/a=5
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5


b/a=6
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5

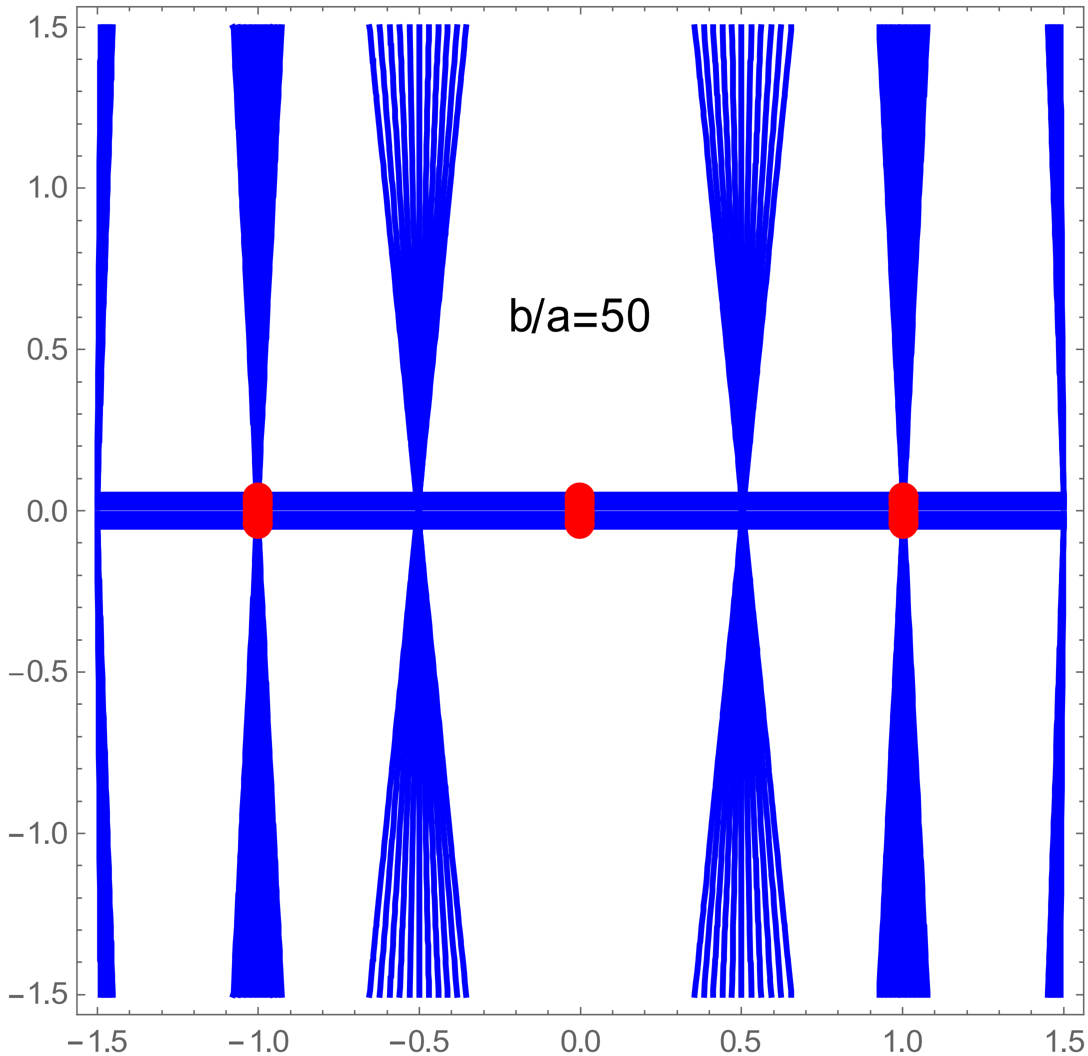


REFERENCES

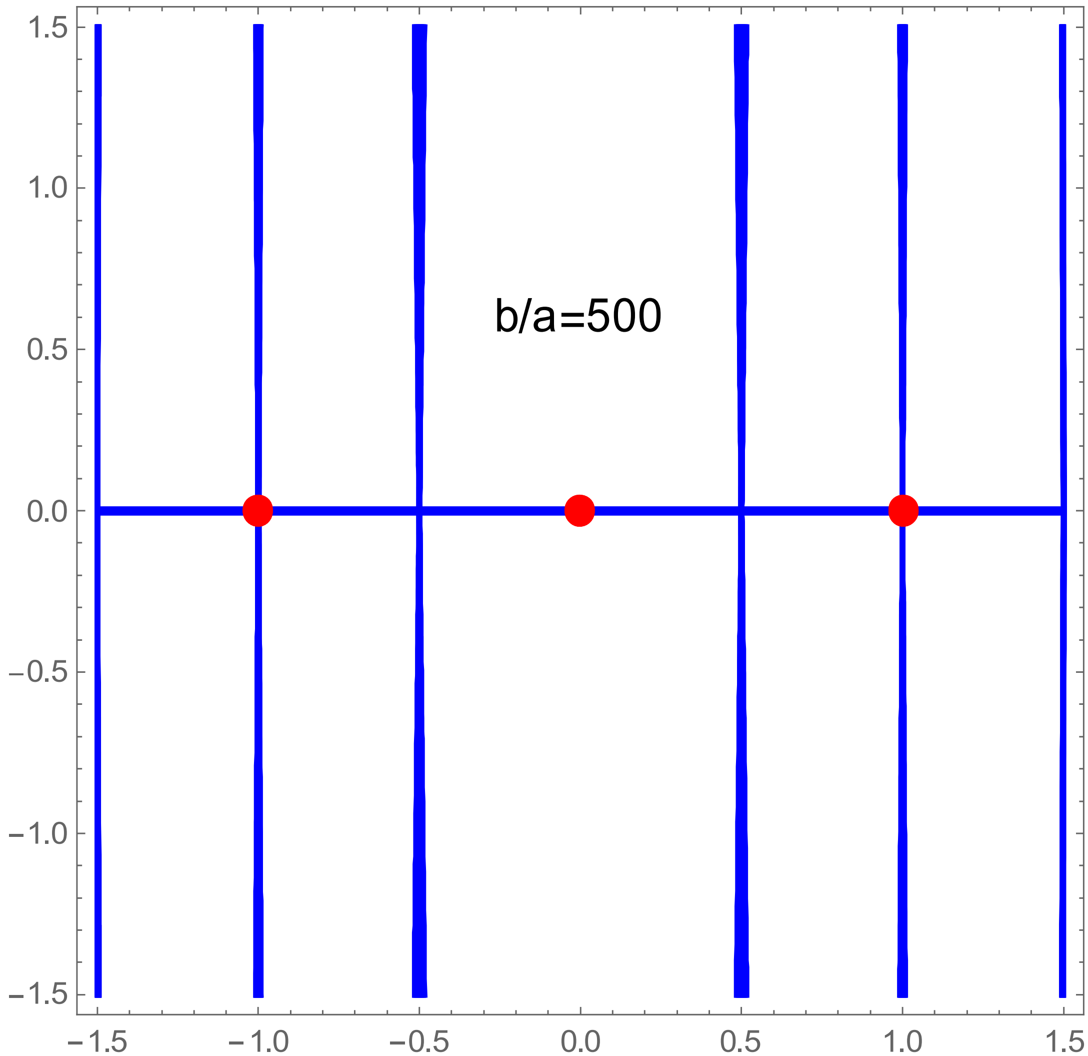
C. Kittel, Introduction to Solid State Physics, 8-th edition (John Wiley & Sons, 2004).



b/a=20
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5



b/a=50
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5


b/a=500
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5

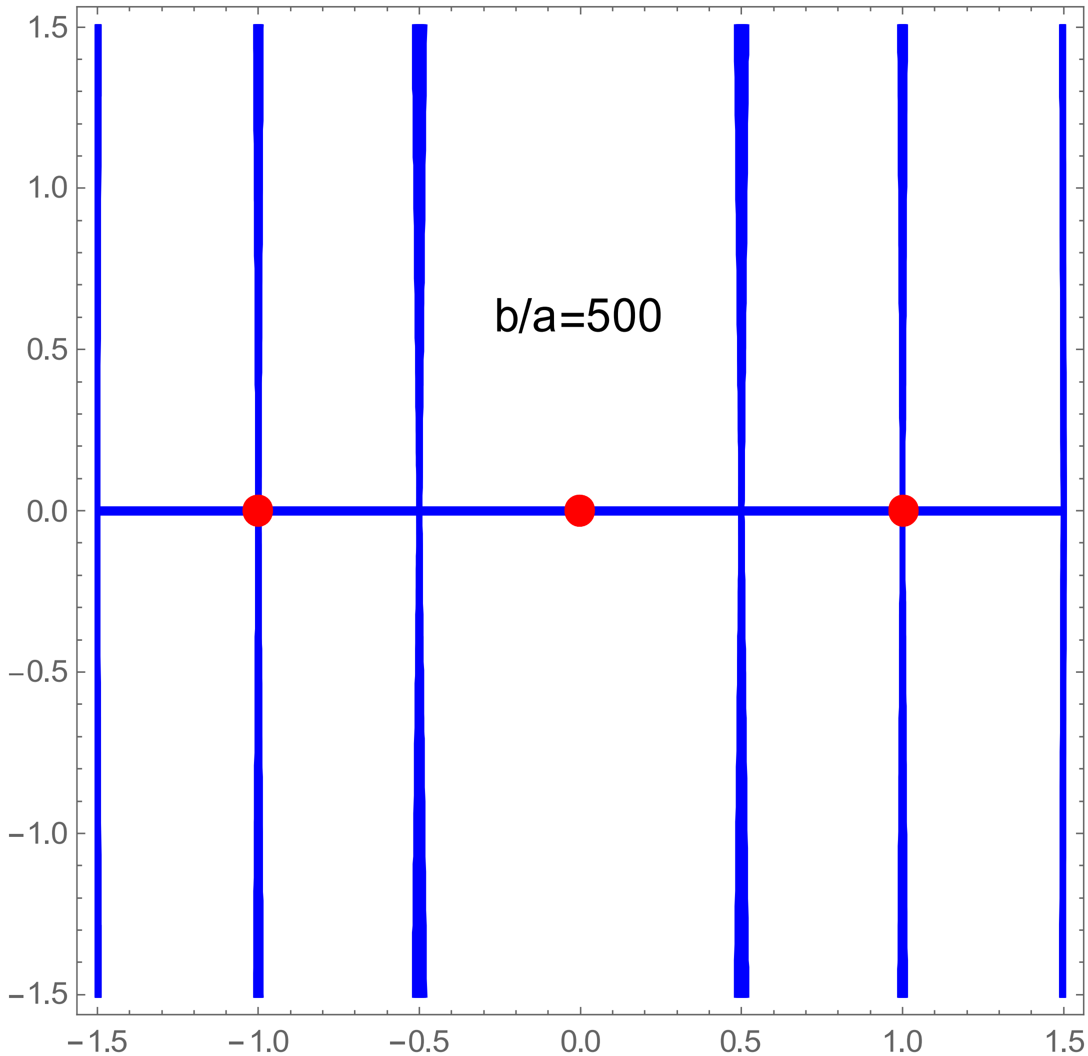
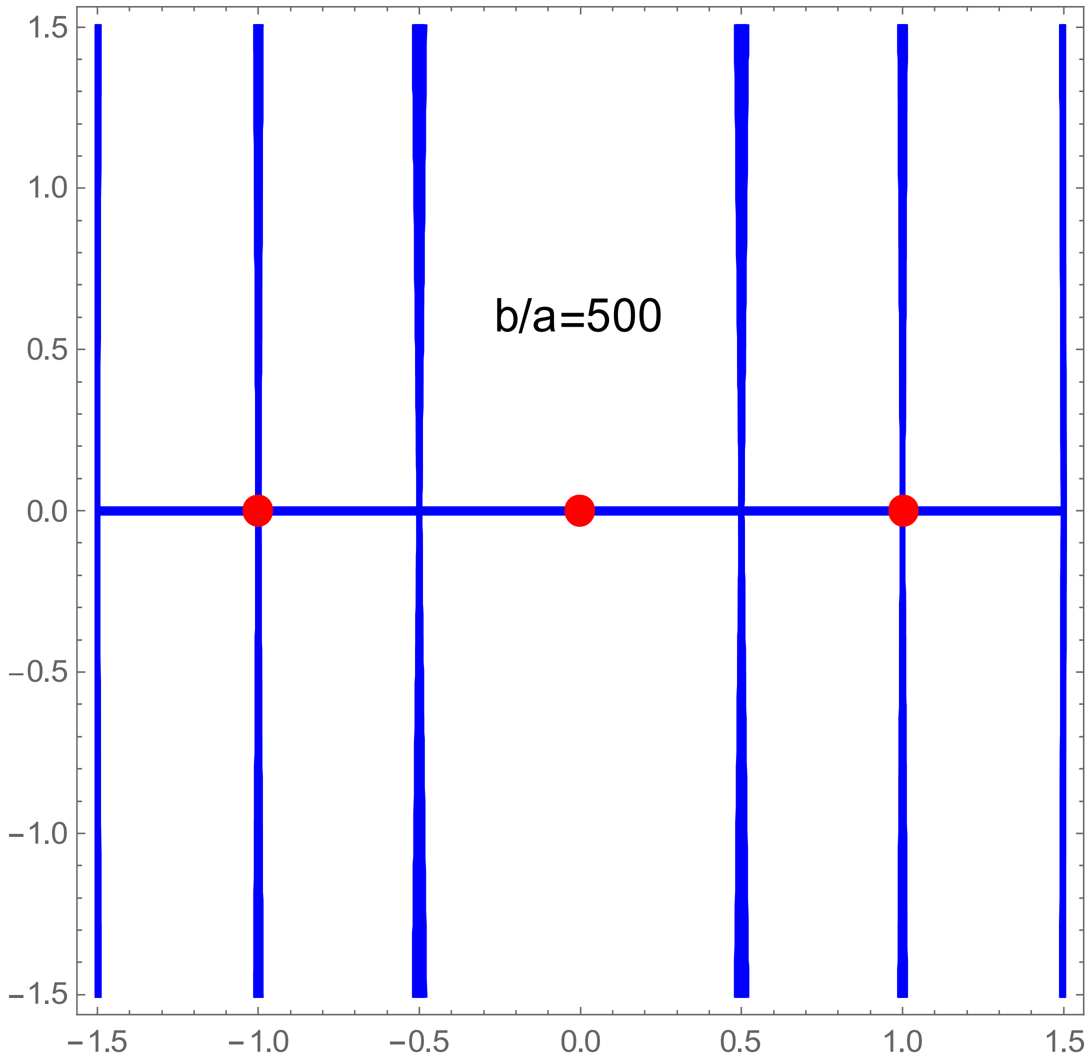


Fig. In the limit of large ratio b/a, the reciprocal lattice



b/a=500
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5