Construction of Fermi surface

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1. Harrison's construction of Fermi surface

There is a way to represent the Fermi surface in the reduced and periodic zone scheme. Fermi surfaces for free electrons are constructed by a procedure credited to Harrison.

The reciprocal lattice points of a square lattice are determined, and free-electron sphere of radius appropriate to the electron concentration is drawn around each point. Any point in ***k*** space that lies within at least one sphere corresponds to an occupied state in the first zone. Points within at least two spheres correspond to occupied states in the second zone, and similarly for points in three or more spheres. In other words, the darker the shading, the higher the zone number.

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2. 2D square lattice

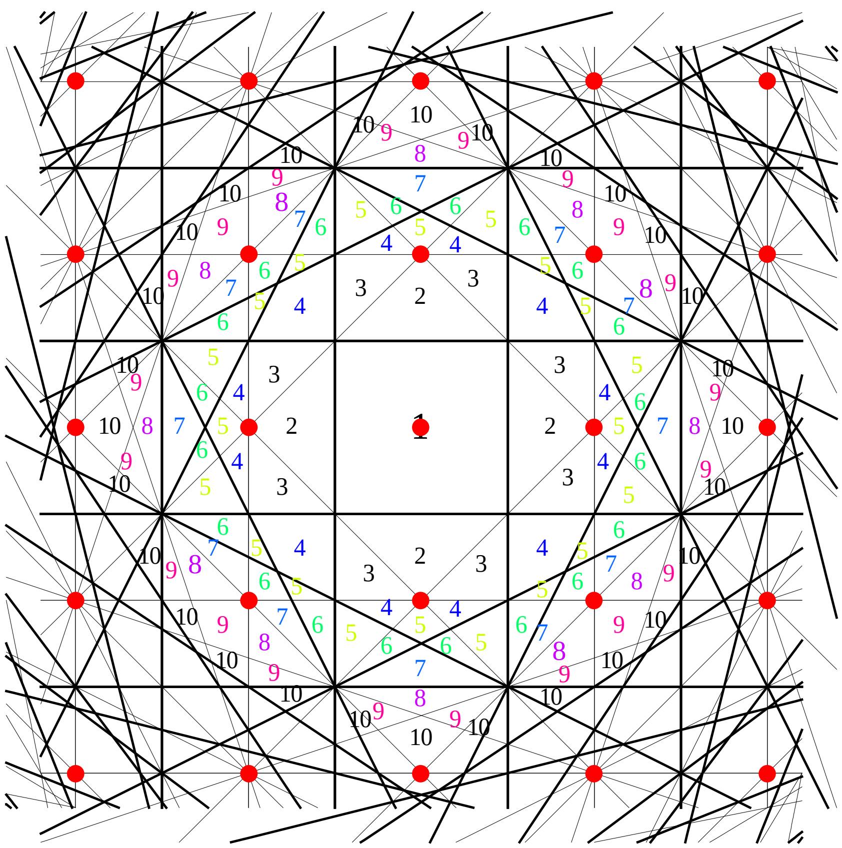

Fig. Brillouin zone for the 2D square lattice.

We assume that there is only one atom per square lattice. Each atom has *p* electrons. Then we get

$$2\frac{L^2}{(2\pi)^2}\pi k_F{}^2 = \frac{L^2}{a^2} p = N\ ,$$

or

$$k_F{}^2 = \frac{2\pi}{a^2} p = \left(\frac{\pi}{a}\right)^2 \frac{2p}{\pi}\ ,$$

or

$$k_F = \sqrt{\frac{2p}{\pi}}\frac{\pi}{a}\,.$$

Note that the Fermi energy is given by

$$\varepsilon_F = \frac{\hbar^2}{2m} k_F{}^2 = \frac{\hbar^2}{2m}(\frac{\pi}{a})^2 \frac{2p}{\pi} = E_0 \frac{2p}{\pi}$$

where

$$E_0 = \frac{\hbar^2}{2m}(\frac{\pi}{a})^2$$

Table: $\frac{k_F}{\pi / a}$ vs p and $\frac{\varepsilon_F}{E_0}$ vs p

p	$k_F/(\pi/a)$	ϵ/E_0
1.	0.797885	0.63662
2.	1.12838	1.27324
3.	1.38198	1.90986
4.	1.59577	2.54648
5.	1.78412	3.1831
6.	1.95441	3.81972
7.	2.111	4.45634
8.	2.25676	5.09296
9.	2.39365	5.72958
10.	2.52313	6.3662

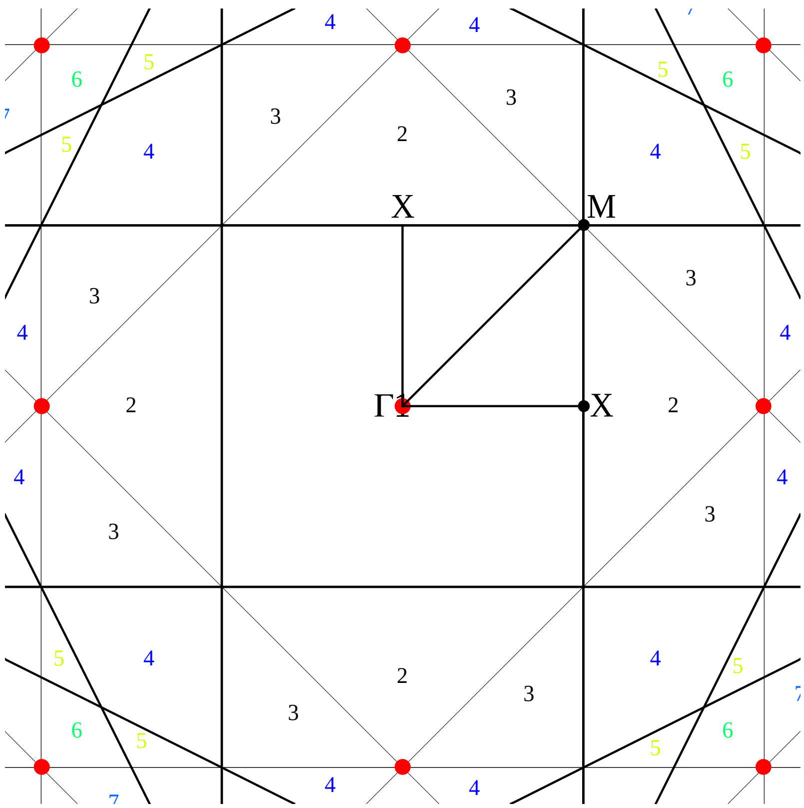

Fig. The Brillouin zone of a 2D square lattice, with some points of high symmetry labelled. $\Gamma X = \pi/a$. $\Gamma P = \sqrt{2}\,\pi/a$

(a) $p = 1$

$$k_F = \sqrt{\frac{2}{\pi}}\frac{\pi}{a} = 0.797885\frac{\pi}{a}.$$

The radius k_F of the Fermi circle is shorter than the length ΓX. The Fermi circle does not contact the zone boubary of the first Brillouin zone.

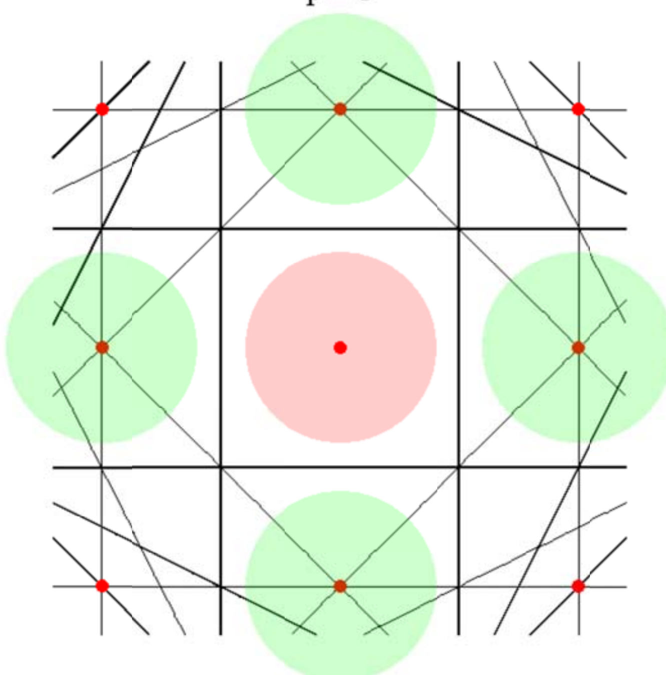

Fig. The 2D Fermi circles corresponding to $p = 1$ electron per atom drawn within the first Brillouin zone structure. Each Brillouin zone is separated by straight lines.

(b) $p = 2$

$$k_F = \sqrt{\frac{4}{\pi}}\frac{\pi}{a} = 1.12838\frac{\pi}{a}.$$

The radius k_F of the Fermi circle is a little longer than the length ΓX. The Fermi circle intersects the zone boudary of the first Brillouin zone around the point X. A part of the

Fermi circle passes the region of the second Brillouin zone. The Harrison;s construction of the Fermi surface is shown below.

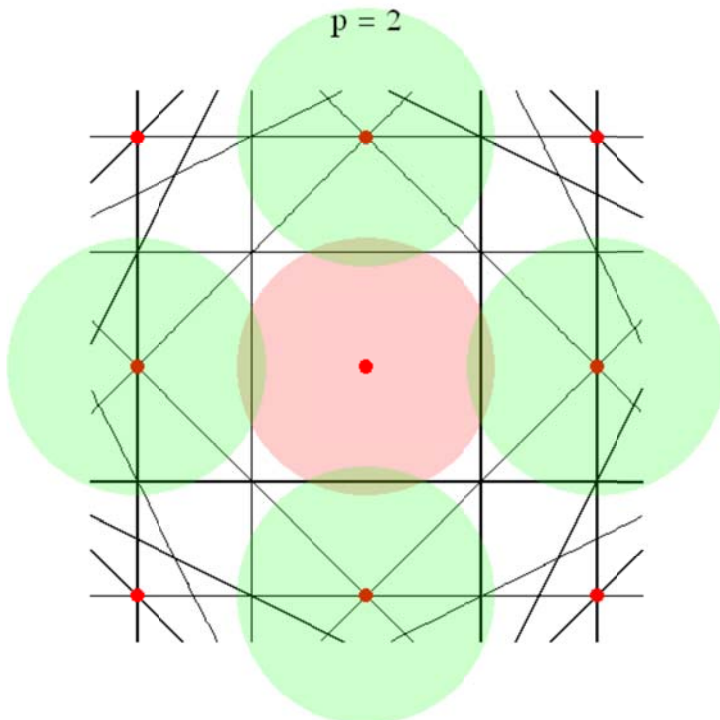

Fig. Harrison construction of free electron Fermi surfaces. The 2D Fermi circles corresponding to $p = 2$ electron per atom.

(i) Hole-like Fermi surface (the first Brillouin zone)

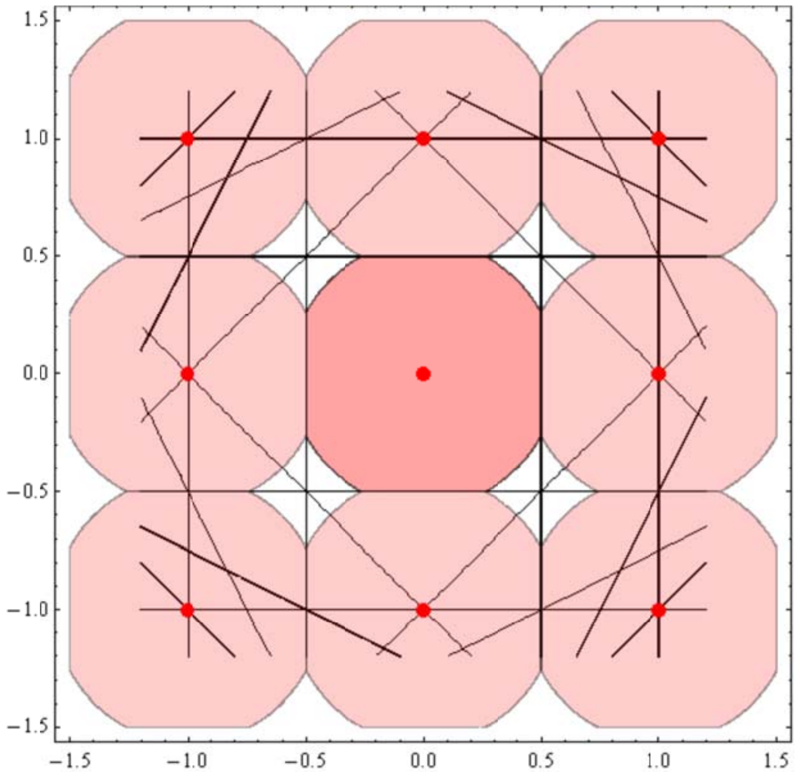

Fig. The Fermi surface in the first Brillouin zone (the periodic zone scheme). $p = 2$. The shaded areas contain electrons, froming a hole-like Fermi surface at each corner of the Brillouin zone (the point M).

(ii) Electron-like Fermi surface in the second Brillouin zone

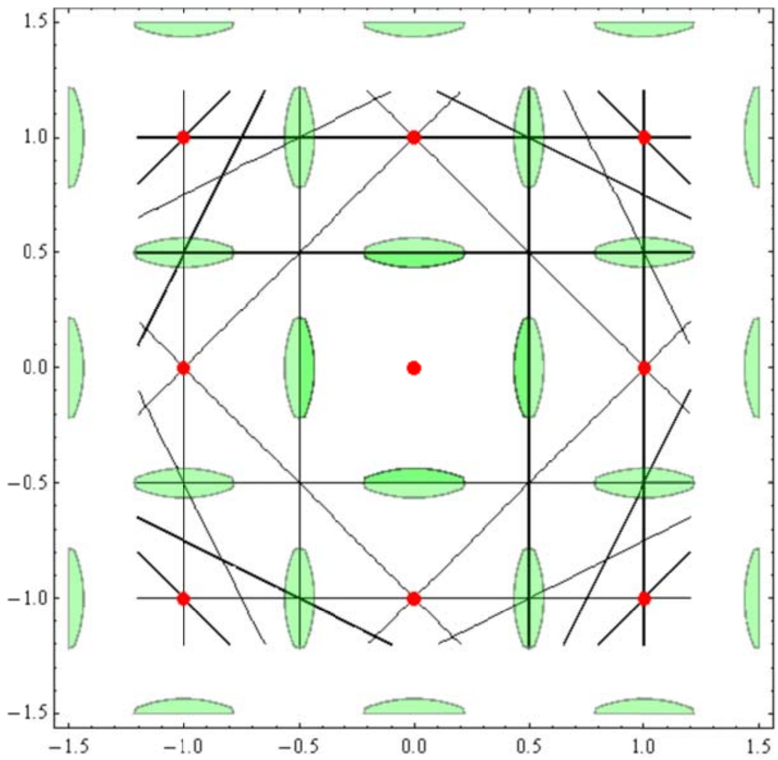

Fig. The Fermi surface in the second Brillouin zone (the periodic zone scheme). The shaded areas contain electrons. $p = 2$. This shaded area (green) forms an electron-like Fermi surface.

(c) $p = 3$

$$k_F = \sqrt{\frac{6}{\pi}}\frac{\pi}{a} = 1.38198\frac{\pi}{a}.$$

The radius k_F of the Fermi circle is longer than the length ΓX, but is slightly shorter than the length ΓM. The Fermi circle passes through the region of the second Brillouin zones and a very small part of the first Brillouin zone. The Harrison's construction of the Fermi surface is shown below.

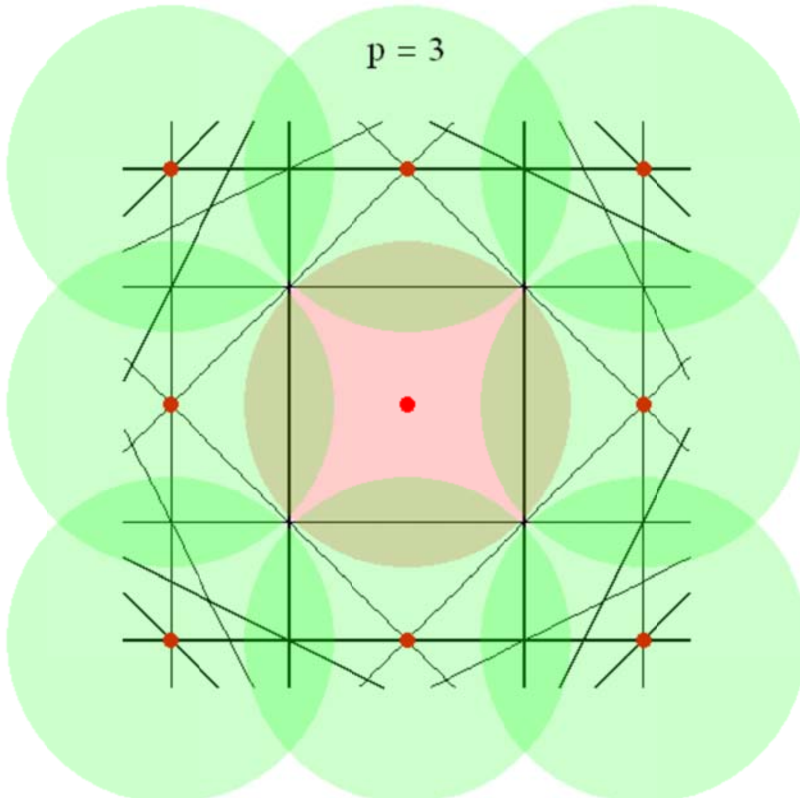

Fig. Harrison construction of free electron Fermi surfaces. The 2D Fermi circles corresponding to $p = 3$ electron per atom. *The first zone is almost full*.

Electron-like Fermi surface (the second zone)

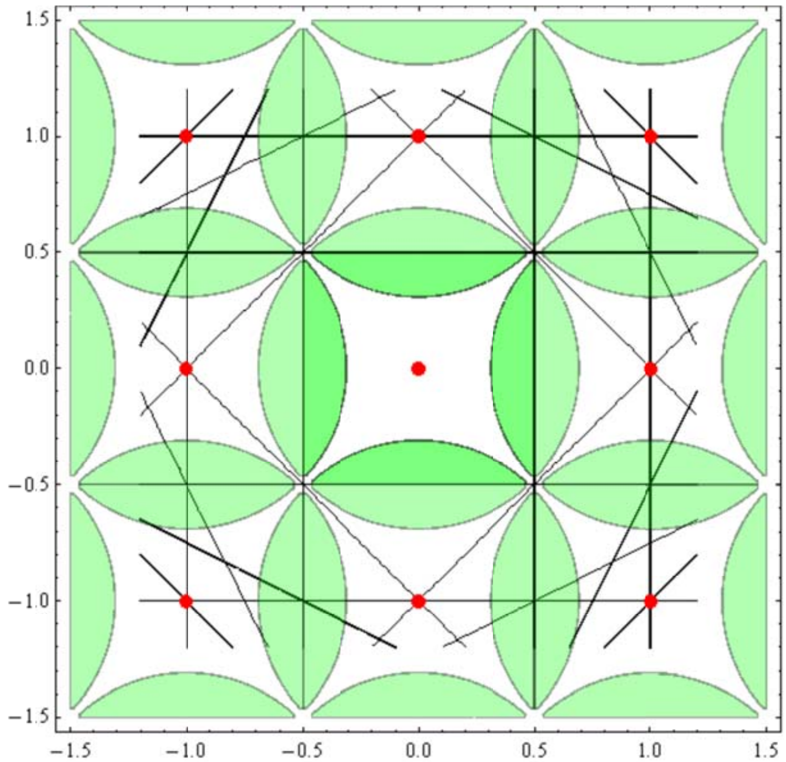

Fig. The Fermi surface in the second zone. p = 3. The shaded areas contain electrons. The Fermi surface is electron-like.

(c) p = 4

$$k_F = \sqrt{\frac{8}{\pi}}\frac{\pi}{a} = 1.59577\frac{\pi}{a}.$$

The radius k_F of the Fermi circle is much longer than the length ΓX, and is longer than the length ΓM. The Fermi circle passes through the region of the second, third, and fourth Brillouin zones. The Harrison's construction of the Fermi surface is shown below.

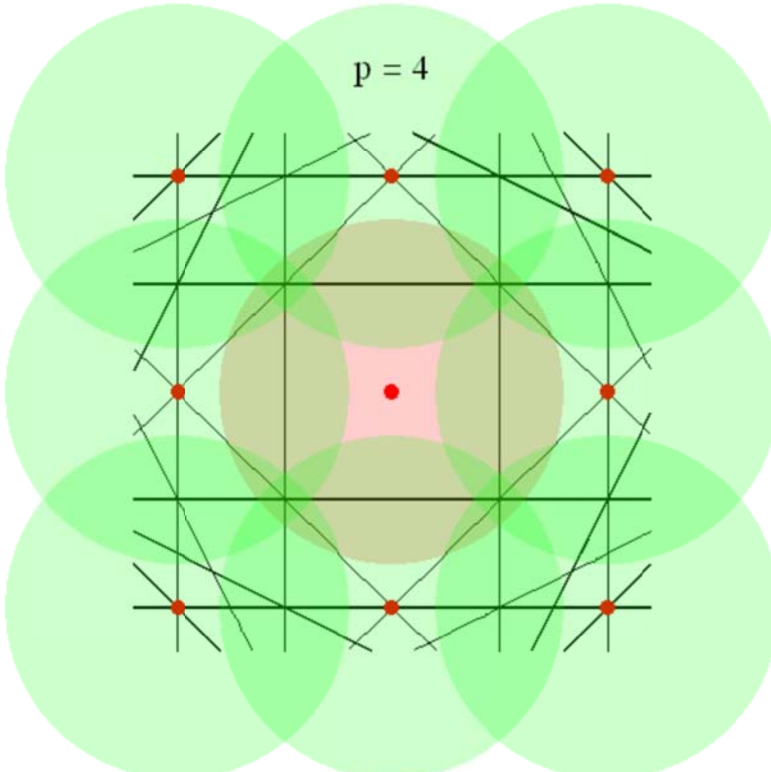

Fig. Harrison construction of free electron Fermi surfaces. The 2D Fermi circles corresponding to p = 4 electrons per atom. *The first zone is completely full*. A circle is drawn around each reciprocal lattice point. Any point in k-space that lies within at least one circle corresponds to an occupied state in the first zone. Points within at least two circles correspond to occupied states in the second zone. Note that each Fermi surface is uniquely determined by the number of overlapping circles.

(i) Hole-like surface in the second Brillouin zone

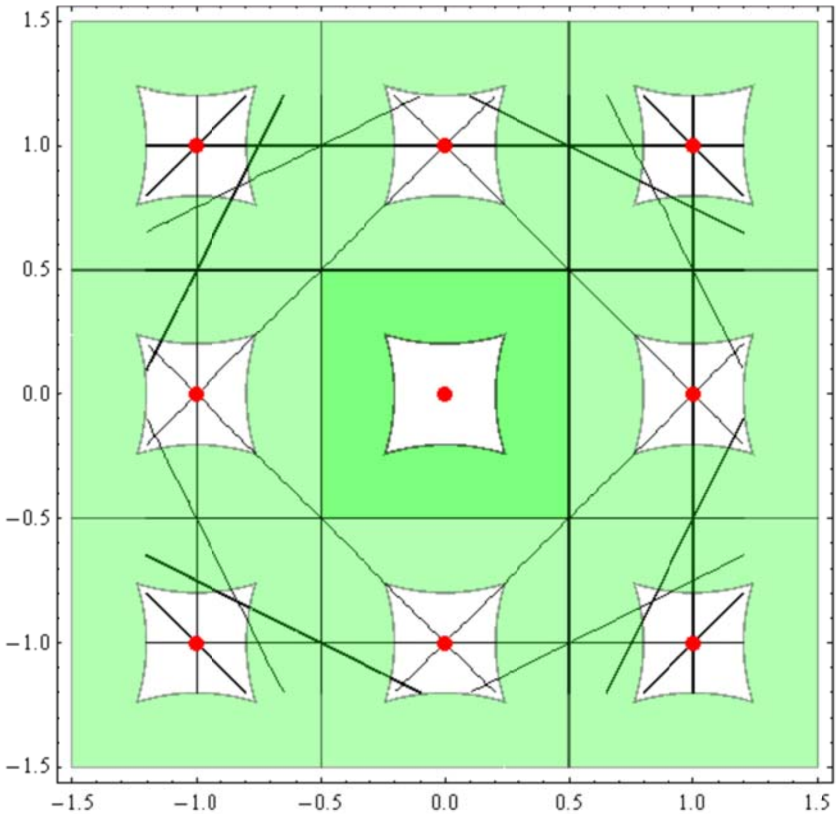

Fig. The Fermi surface in the second zone. p =4 (periodic zone scheme). The shaded area represents occupied electron states. The Fermi surface is *hole-like*.

(ii) Electron-like Fermi surface (the third Brillouin zone)

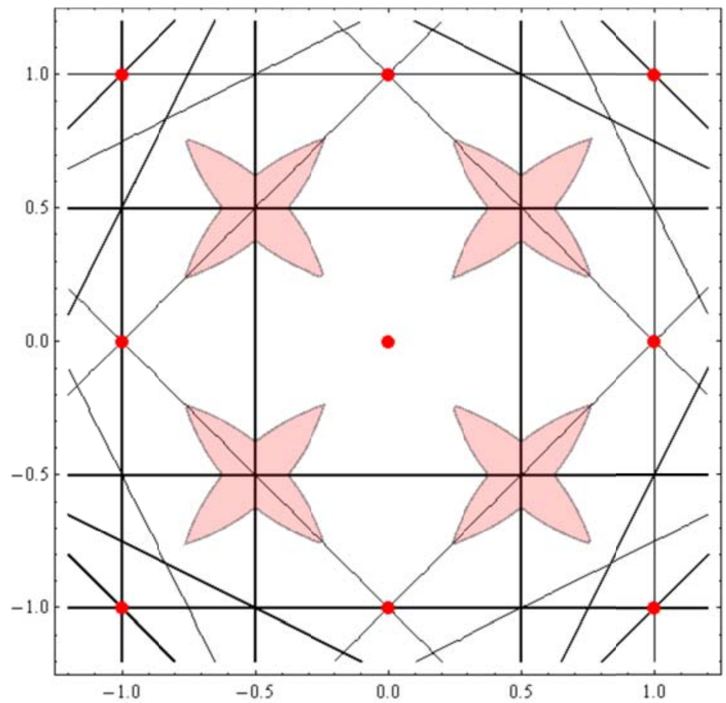

Fig. The Fermi surface in the third zone (the periodic zone scheme). p = 4. The shaded area represents occupied electron states. The Fermi surface is *electron-like*.

(iii) Electron-like Fermi surface (the fourth Brillouin zone).

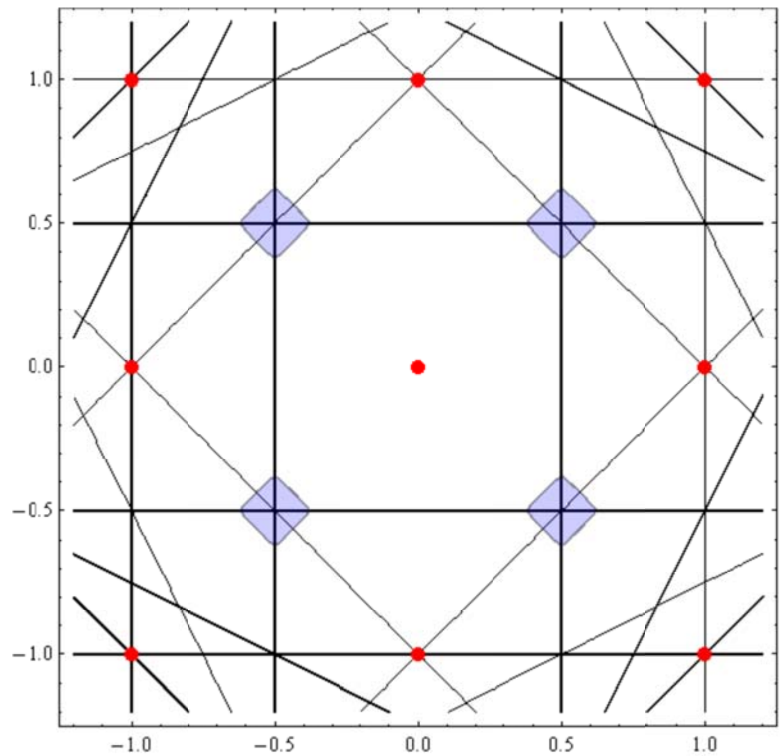

Fig. The Fermi surface in the fourth zone (periodic zone scheme). p = 4. The shaded area represents occupied electron states, forming the electron-like Fermi surface.

(e) ***p*** **= 5**

$$k_F = \sqrt{\frac{10}{\pi}}\frac{\pi}{a} = 1.78412\frac{\pi}{a}$$

The Fermi circle passes through the region of the second, third, and fourth Brillouin zones. The Harrison's construction of the Fermi surface is shown below.

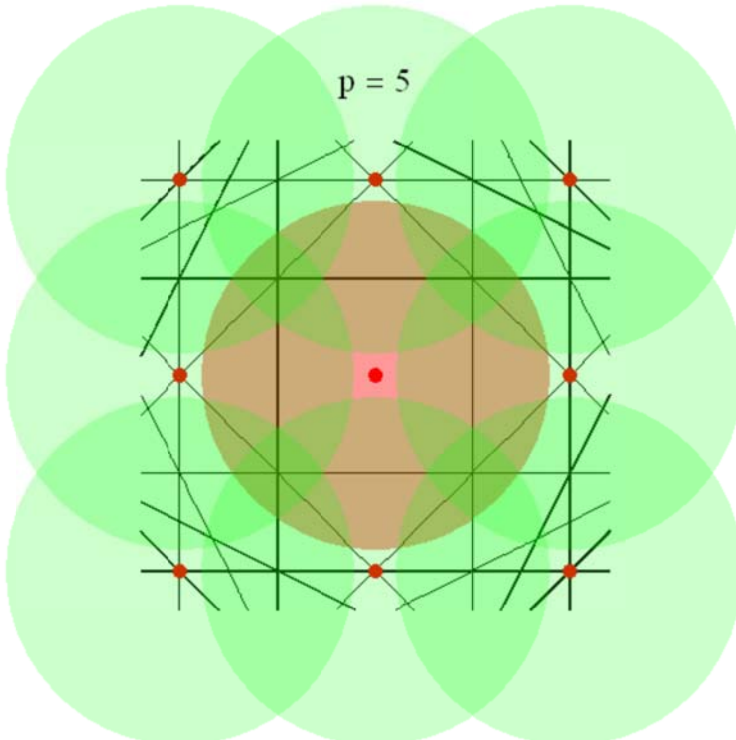

Fig. Harrison construction of free electron Fermi surfaces. The 2D Fermi circles corresponding to $p = 5$ electron per atom. The first zone is completely full.

(i) Hole-like Fermi surface (the second Brillouin zone)

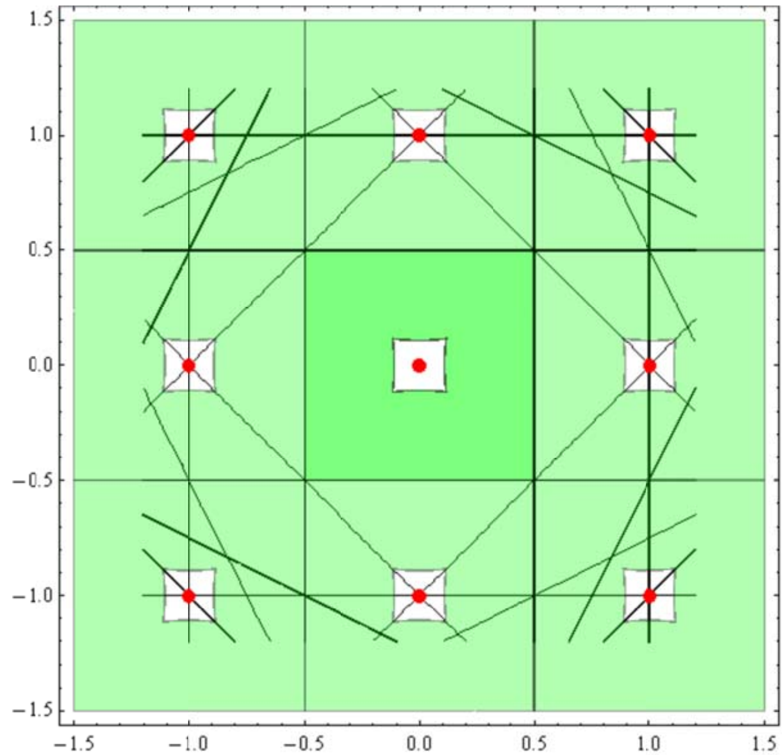

Fig. The Fermi surface in the second zone. p =5 (periodic zone scheme). The shaded area represents occupied electron states. T*he Fermi surface is hole-like. The first zone is completely full*.

(ii) Electron-like Fermi surface (the third Brillouin zone)

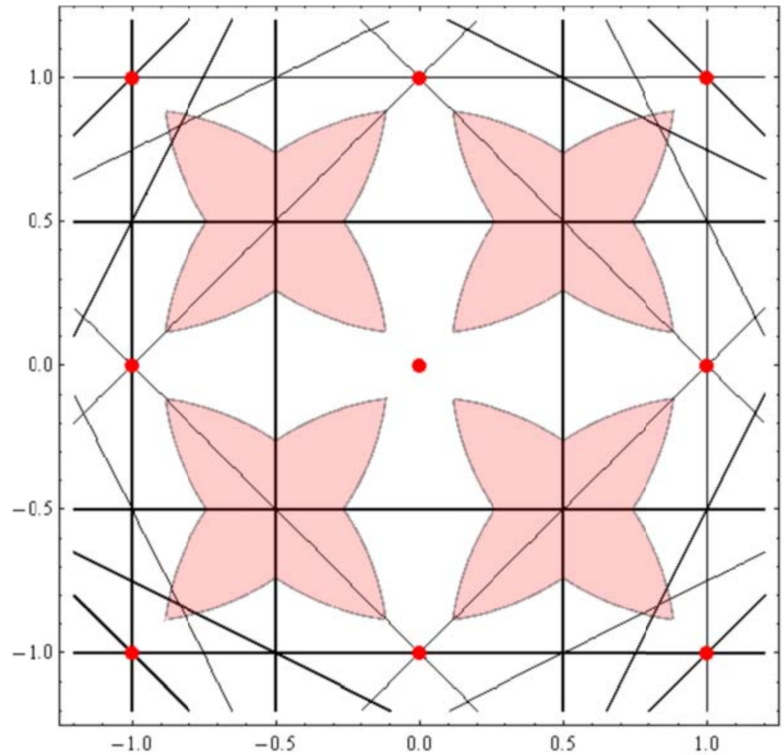

Fig. The Fermi surface in the third zone (the periodic zone scheme). $p = 5$. The shaded area represents occupied electron states. *The Fermi surface is electron-like*.

(iii) Hole-like Fermi surface (the fourth Brillouin zone)

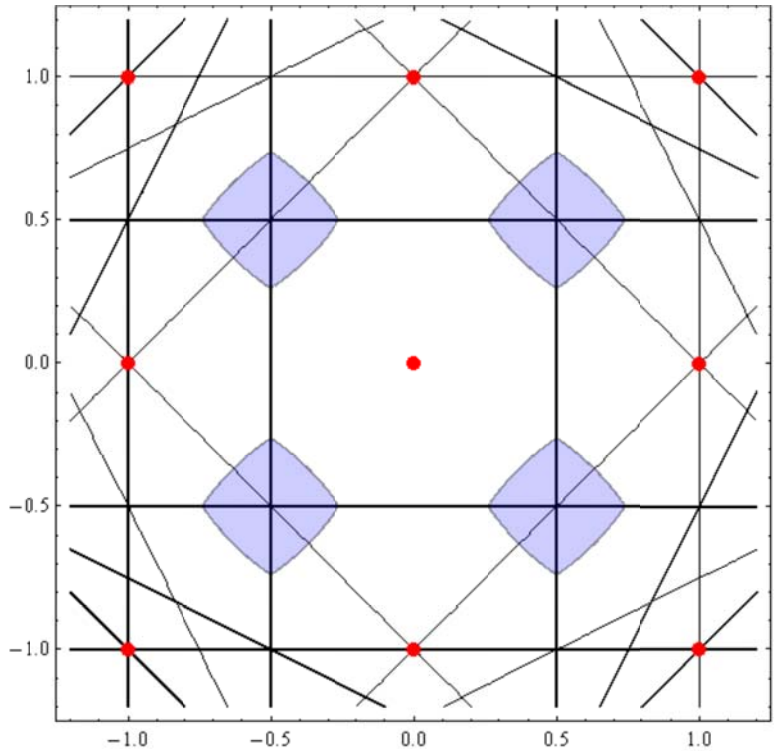

Fig. The Fermi surface in the fourth zone (periodic zone scheme). $p = 5$. The shaded area represents occupied electron states, forming the *electron-like Fermi surface*.

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3. 2D hexagonal lattice metal

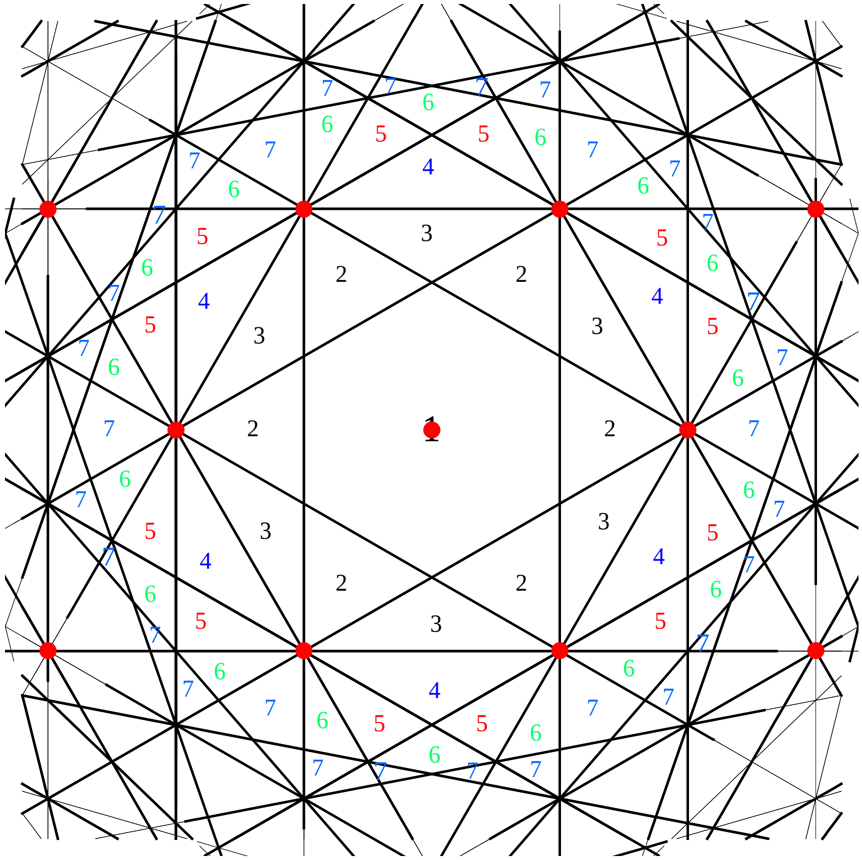


Fig. The Brillouin zones for a 2D hexagonal lattice.

We assume that there is one atom per area $\frac{\sqrt{3}a^2}{2}$. Each atom has p electrons. Then we get

$$2\frac{A}{(2\pi)^2}\pi k_F{}^2 = \frac{A}{\frac{\sqrt{3}a^2}{2}}p\,,$$

Then k_F is calculated as

$$k_F = \frac{2\sqrt{\pi p}}{3^{1/4}a},$$

The Fermi energy is given by

$$\varepsilon_F = \frac{\hbar^2}{2m} k_F{}^2 = \frac{\hbar^2}{2m} [\frac{2\sqrt{\pi p}}{3^{1/4} a}]^2 = \frac{\hbar^2}{2m} \left(\frac{\pi}{a}\right)^2 (\frac{4p}{3^{1/2}\pi}) = E_0 (\frac{4p}{3^{1/2}\pi})$$

where

$$E_0 = \frac{\hbar^2}{2m} \left(\frac{\pi}{a}\right)^2$$

Note that the reciprocal lattice vector is given by

$$G_1 = \frac{4\pi}{\sqrt{3}a}.$$

The ratio k_F to the zone boundary of the first Brillouin zone (G/2) is

$$\frac{k_F}{G_1/2} = 3^{1/4} \sqrt{\frac{p}{\pi}} = 0.742515\sqrt{p}\ .$$

For $p = 1$, this ratio is smaller than 1, while for $p \geq 2$, this ratio is larger than 1. This means that for $p = 1$, there is a Fermi circle inside the first Brillouin zone. We also calculate

$$\frac{k_F}{G_1/\sqrt{3}} = \sqrt{3}\frac{k_F}{G_1} = \frac{1}{2} 3^{3/4} \sqrt{\frac{p}{\pi}}$$

Table

p	$k_F/(G_1/2)$	$k_F/(G_1/\sqrt{3})$	ϵ/E_0
1.	0.742515	0.643037	0.735105
2.	1.05008	0.909392	1.47021
3.	1.28607	1.11377	2.20532
4.	1.48503	1.28607	2.94042
5.	1.66031	1.43787	3.67553
6.	1.81878	1.57511	4.41063
7.	1.96451	1.70132	5.14574
8.	2.10015	1.81878	5.88084
9.	2.22755	1.92911	6.61595
10.	2.34804	2.03346	7.35105

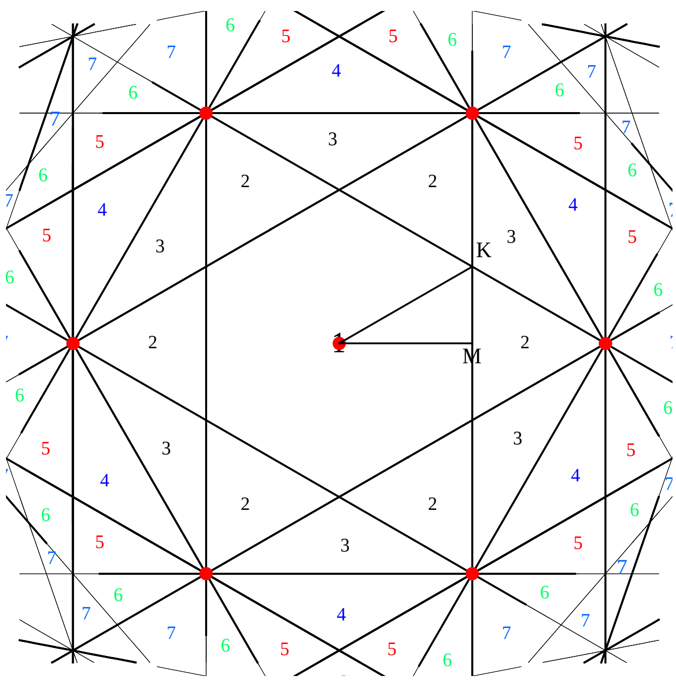


Fig. Brillouin zones for the 2D hexagonal lattice with some points of high symmetry labelled. $\Gamma M = \frac{G_1}{2}$. $\Gamma K = \frac{G_1}{\sqrt{3}}$. G_1 (= $\frac{4\pi}{\sqrt{3}a}$) is the reciprocal lattice

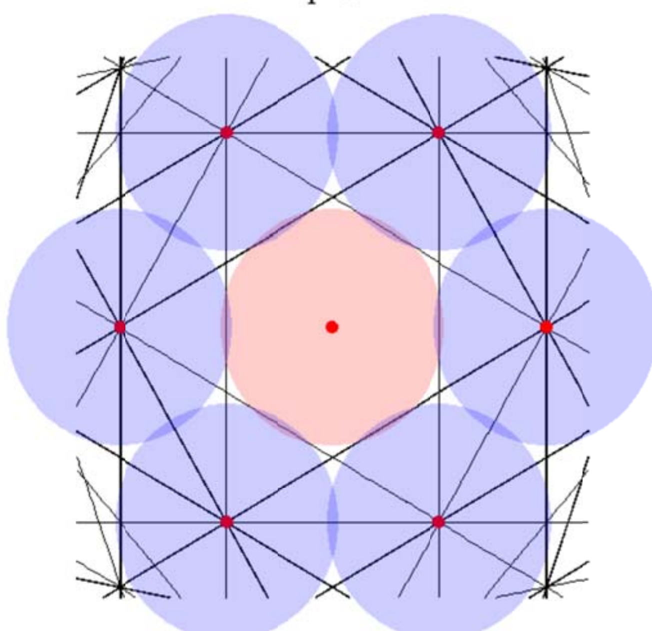
Here we apply the Harrison's construction of Fermi surfaces to the case of 2D hexagonal lattice where $p \geq 2$.

(a) $p = 2$

$$\frac{k_F}{G_1/2} = 1.05008, \qquad \frac{k_F}{G_1/\sqrt{3}} = 0.909392$$

The radius k_F of the Fermi circle is a little longer than the shortest length (ΓM)of the first Brillouin zone However, the Fermi circle does not contact the zone corner (the Point K) of the first Brillouin zone. The Fermi circle passes the region of the first and second Brillouin zones. The Harrison's construction of the Fermi surface is shown below.

p=2



(i) Hole-like Fermi surface (the first Brillouin zone).

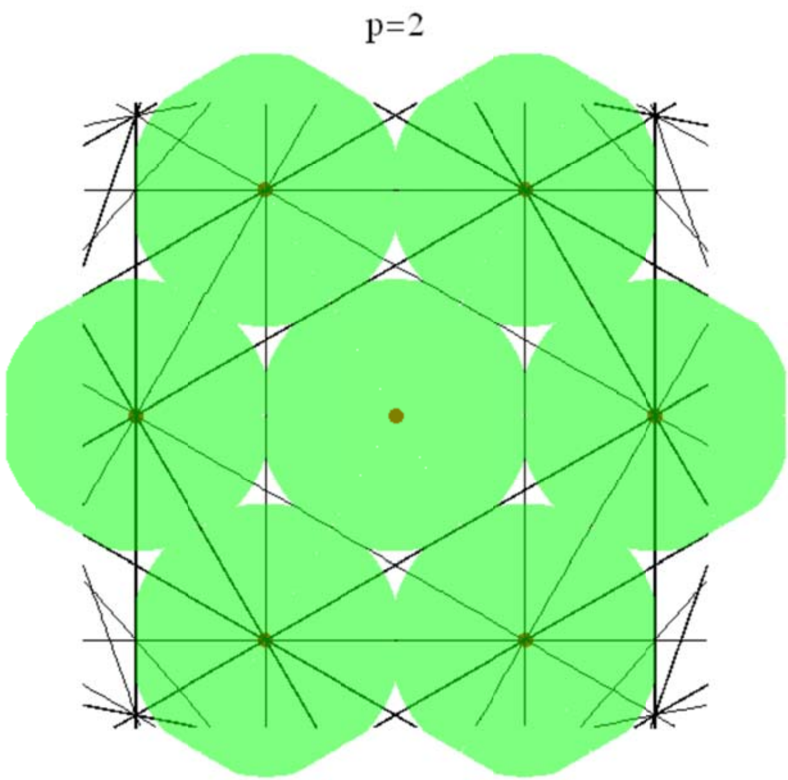


Fig. The Fermi surface in the first zone (periodic zone scheme). $p = 2$. The shaded area represents occupied electron states, forming a hole-like Fermi surface.

(ii) The electron-like Fermi surface (the second Brillouin zone)

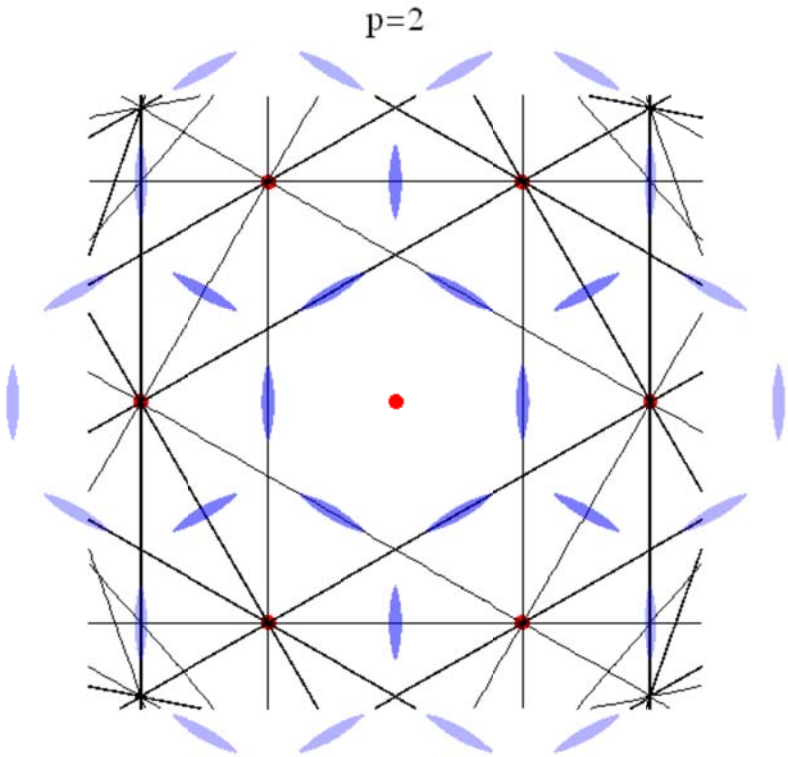


Fig. The Fermi surface in the second zone (periodic zone scheme). p = 2. The shaded area represents occupied electron states, forming an electron-like Fermi surface.

(b) $p = 4$

$$\frac{k_F}{G_1/2} = 1.48503, \qquad \frac{k_F}{\sqrt{3}G_1} = 1.28607$$

The Fermi circle passes outside the zone corner (the point K) of the first Brillouin zone. The first zone is completely full. The Harrison's construction of the Fermi surface is shown below.

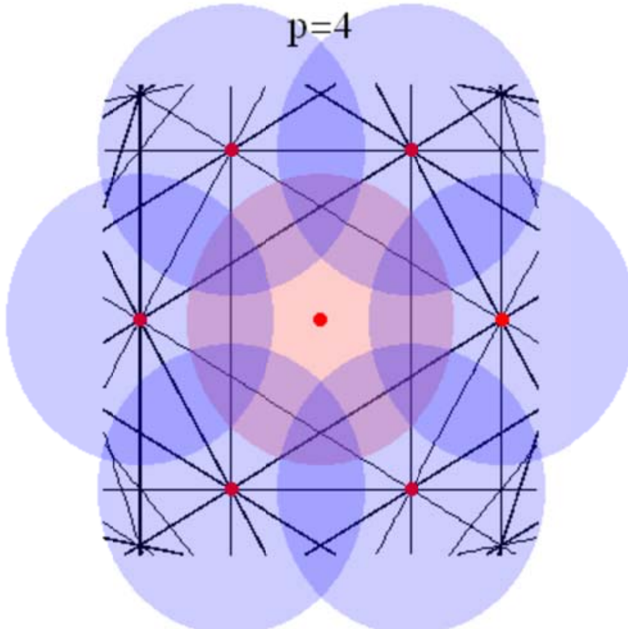


Fig. Harrison's construction of Fermi surfaces for the 2D hexagonal lattice. p =4.

(i) The hole-like Fermi surface (the second zone)

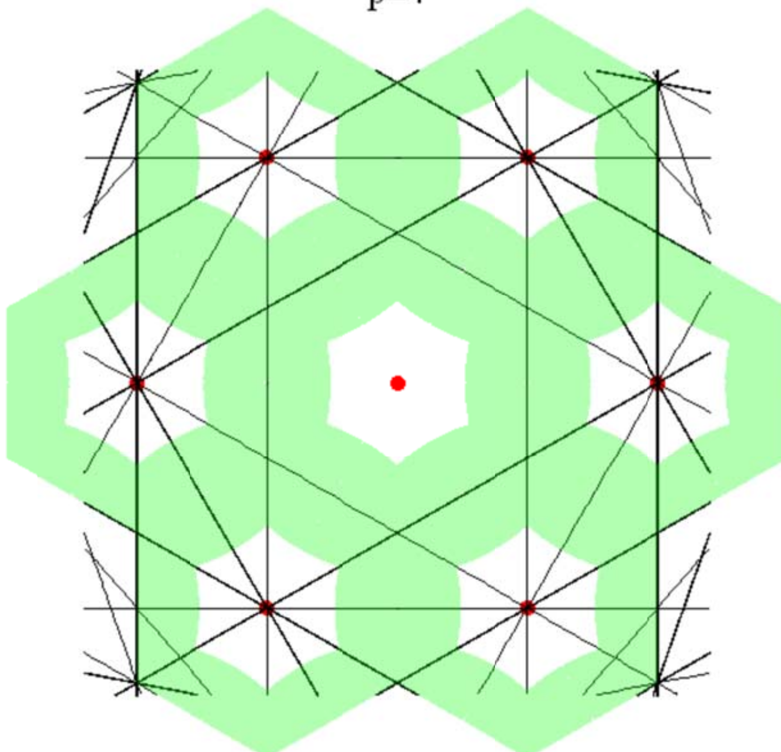


Fig. The Fermi surface in the second zone (periodic zone scheme). p = 4. The shaded area represents occupied electron states, forming a hole-like Fermi surface.

(ii) The electron-like Fermi surface (the third zone)

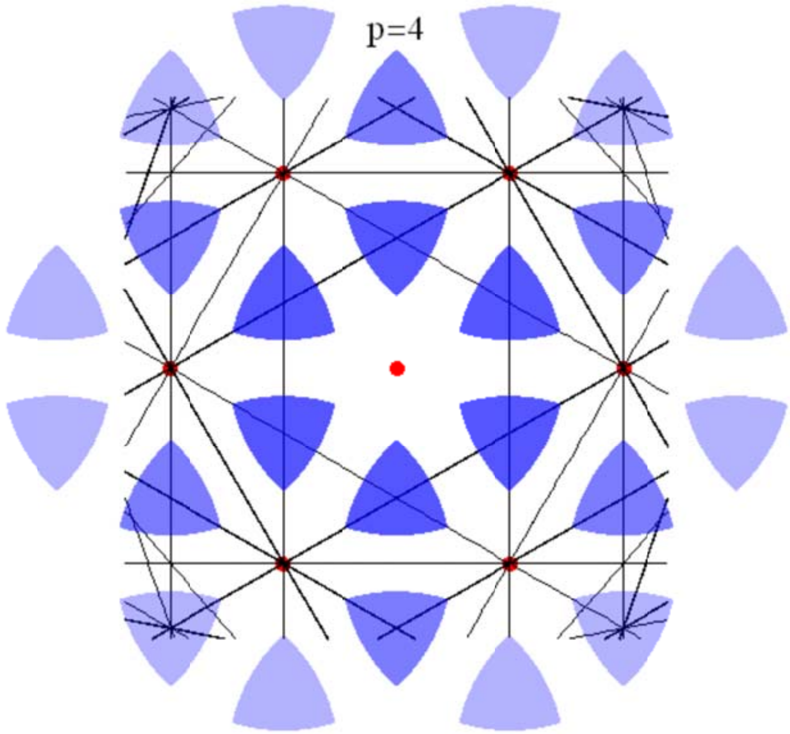


Fig. The Fermi surface in the third zone (periodic zone scheme). p = 4. The shaded area represents occupied electron states, forming an electron-like Fermi surface.

(c) $p = 6$

$$\frac{k_F}{G_1/2} = 1.81878\,, \qquad \frac{k_F}{\sqrt{3}G_1} = 1.57511$$

The first zone is completely full. The Fermi circle passes through the secod, third, and fourth Brillouin zones. The Harrison's construction of the Fermi surface is shown below.

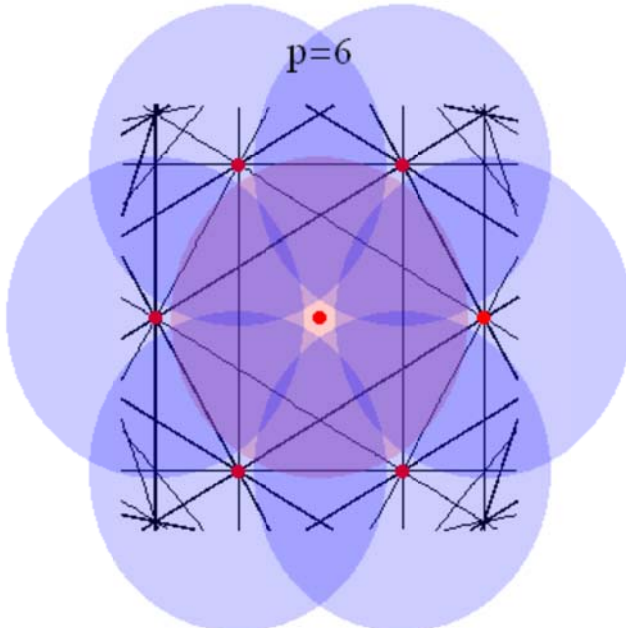


Fig. Harrison's construction of Fermi surfaces for the 2D hexagonal lattice. p =6.

(i) Hole-like Fermi surface (the second zone)

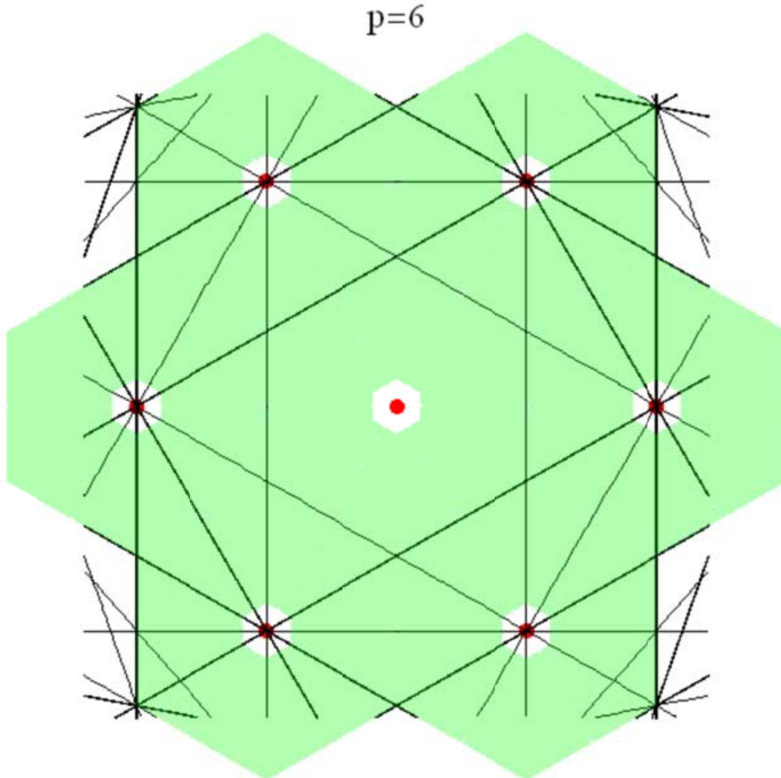


Fig. The Fermi surface in the second zone (periodic zone scheme). p = 6. The shaded area represents occupied electron states, forming a hole-like Fermi surface.

(ii) Hole-like Fermi surface (the third zone)

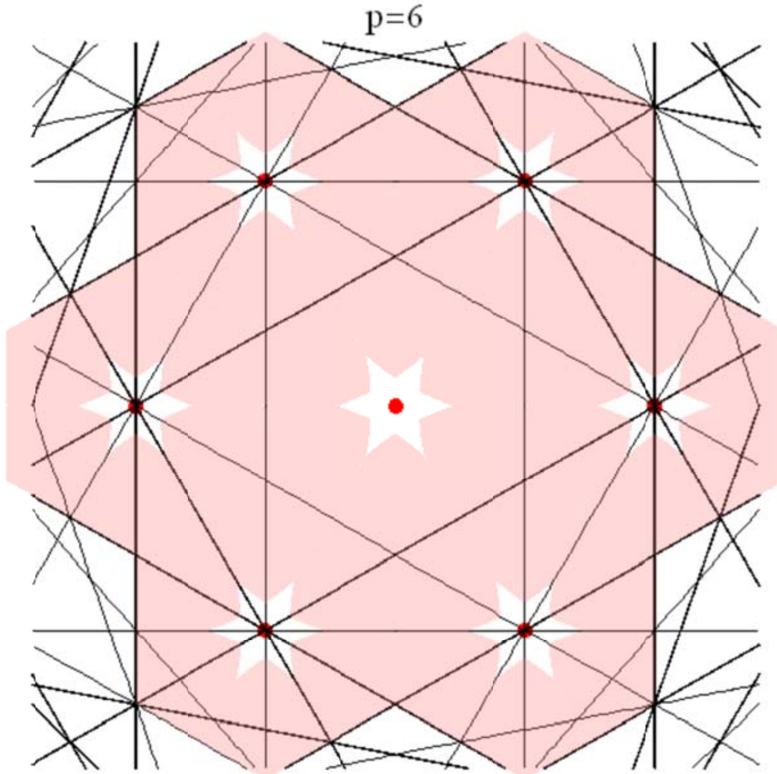


Fig. The Fermi surface in the third zone (periodic zone scheme). p = 6. The shaded area represents occupied electron states, forming a hole-like Fermi surface.

(iii) Electron-like Fermi surface (the fourth zone)

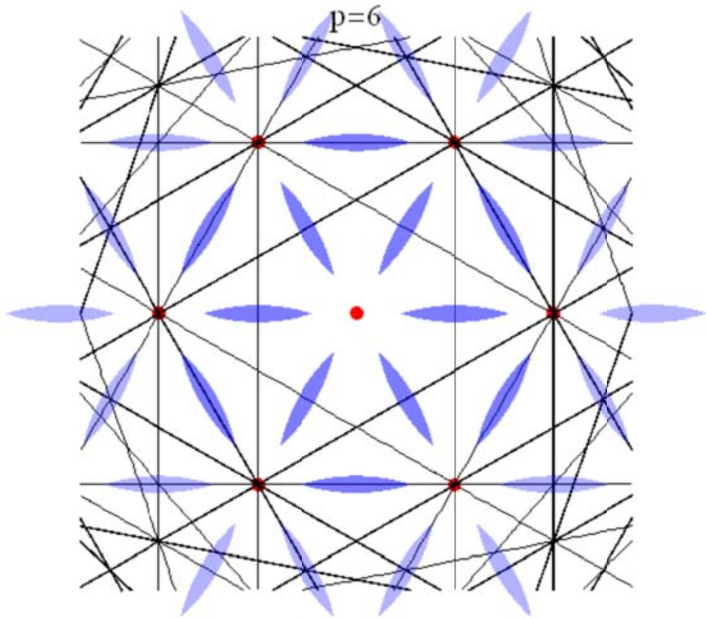


Fig. The Fermi surface in the fourth zone (periodic zone scheme). p = 6. The shaded area represents occupied electron states, forming an electron-like Fermi surface.

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