I. A two-dimensional free-electron gas.

1. Using the 2-dimensional Schrödinger equation, show that the wave function and energy band are :

$$\psi_{\vec{k}}(\vec{x}) = B\mathrm{e}^{ik_x x}\mathrm{e}^{ik_y y}$$
$$E_{\vec{k}} = \frac{\hbar^2\left(k_x^2 + k_y^2\right)}{2m}$$

where m is the mass of the electron, $\vec{k} = (k_x, k_y)$ is the wave vector and B is the normalization constant.

Answer: For 2-D shrödinger Equation:

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\vec{r}) + V\psi(\vec{r}) = E\psi(\vec{r})$$

With V=0

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\vec{r}) = E\psi(\vec{r})$$

The solution of this equation is travelling plane wave:

$$\psi(\vec{r}) = Be^{i\vec{k}\cdot\vec{r}} = Be^{i(k_x\cdot x + k_y\cdot y)}$$

($e^{-i\vec{k}\cdot\vec{r}}$ term may be absorbed into the direction of $\vec{k}$)
And

$$E_{\vec{k}} = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2\left(k_x^2 + k_y^2\right)}{2m}$$

2. By a simple integration over the square of side L, find the constant B

Answer:

$$\psi(\vec{r}) = Be^{i\vec{k}\cdot\vec{r}} = Be^{i(k_x\cdot x + k_y\cdot y)}$$
$$\int_0^L \psi(\vec{r}) = 1$$
$$\int_0^L dx \int_0^L dy|\psi(\vec{r})|^2 = 1$$
$$B^2 \cdot L^2 = 1$$
$$B = \frac{1}{L}$$

3. Express clearly the allowed values of $\vec{k}$. How many states are in the elementarybox :$\Delta k_x \Delta k_y = (2\pi/L)^2$?

Answer: According to PBC,

$$\psi_k(x+L,y) = \psi_k(x,y), \quad \psi_k(x,y+L) = \psi_k(x,y)$$

$$\text{So for x, we have} \quad \frac{1}{L}e^{i(k_x\cdot(x+L)+k_y\cdot y)} = \frac{1}{L}e^{i(k_x\cdot x+k_y\cdot y)}$$

$$\Downarrow$$

$$e^{ik_x\cdot x} = 1$$

$$\Downarrow$$

$$k_x = \frac{2\pi}{L}n_x, \quad n_x = 0, \pm1, \pm2\cdots$$

$$\text{Similarly, for y} \quad k_y = \frac{2\pi}{L}n_y, \quad n_y = 0, \pm1, \pm2\cdots$$

$$\text{It is easy to find that:} \quad \Delta k_x = \Delta k_y = \frac{2\pi}{L}$$

As **Figure 1** shows, there is only one grid point in each elementary box $\left(\frac{2\pi}{L}\right)^2$
Of course, if we consider spin, then we have **two** states in such box.

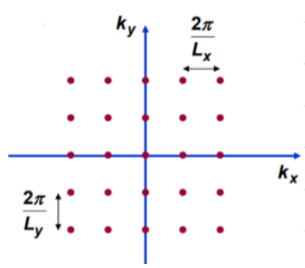

Figure 1: 2-D k space

4. We can also use plane polar coordinates, $\vec{k} = (|\vec{k}|, \varphi)$, so that $k_x = |\vec{k}|\cos\varphi$ and $k_y = |\vec{k}|\sin\varphi$ in the standard way. Show that the energy band is a parabola as a function of $k = |\vec{k}|$

Answer: In the polar coordinates:

$$\begin{aligned} k_x &= |k|\cos\varphi \\ k_y &= |k|\sin\varphi \\ \text{So,}E_k &= \frac{\hbar^2\left(|k|^2\cos^2\varphi + |k|^2\sin^2\varphi\right)}{2m} \\ &= \frac{\hbar^2|\,k|^2}{2m} \end{aligned}$$

5. What is the Fermi surface in this 2-dimensional problem ? Please make a drawing in k-space, and mark clearly the occupied and unoccupied regions.

Answer: The Fermi Surface is when $k_F = \sqrt{\frac{2mE_F}{\hbar^2}}$, as **Figure 3** shows, the grid points inside the circle represent the occupied states(yellow part), while the points outside the circle represent the unoccupied states.

6. We must have N electrons confined in our 2-dimensional box. Calculate the electron density $n = \frac{N}{L^2}$ using the zero-temperature expression :

$$N = 2\sum_{\vec{k}} \theta\left(k_F - |\vec{k}|\right)$$

Compare your answer to the analogous law for the 3-dimensional electron gas.

Answer: Number of electrons is N:

$$\begin{aligned}
N &= 2\sum_{k} \theta\left(k_F - |\vec{k}|\right) \\
&= 2\iint_{|k|<k_F} dn_x dn_y \\
&= 2\iint \frac{Ldk_x}{2\pi}\cdot\frac{Ldk_y}{2\pi} \\
&= \frac{2A}{(2\pi)^2}\iint dk_x dk_y \\
&= \frac{2A}{(2\pi)^2}\iint d|k|\cdot|k|d\varphi \\
&= \frac{2A}{(2\pi)^2}\cdot\pi\cdot|k_F|^2 \\
&= \frac{A}{2\pi}|k_F|^2
\end{aligned}$$

So the electron density is $n = \dfrac{N}{A} = \dfrac{|k_F|^2}{2\pi}$

In 3-D case, the Fermi Surface is a sphere, so

$$\begin{aligned}
N &= 2\iiint dn_x dn_y dn_z \\
&= 2\frac{L^3}{(2\pi)^3}\iiint dk_x dk_y dk_z \\
&= \frac{2L^3}{(2\pi)^3}\cdot\frac{4}{3}\pi k_F^3 \\
&= \frac{V}{3\pi^2}k_F^3
\end{aligned}$$

The electron density is $n = \dfrac{N}{V} = \dfrac{|k_F|^3}{3\pi^2}$