

**I. A two-dimensional free-electron gas.**

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

$$\psi_{\vec{k}}(\vec{x}) = B e^{i k_x x} e^{i k_y y}$$

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

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 Schrödinger 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:

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

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

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

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

**Answer:**

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

$$\int_0^L \int_0^L \psi(\vec{r}) = 1$$

$$\int_0^L dx \int_0^L dy |\psi(\vec{r})|^2 = 1$$

$$B^2 \cdot L^2 = 1$$

$$B = \frac{1}{L}$$

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

**Answer:** According to PBC,

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

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

$$\Downarrow$$

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

$$\Downarrow$$

$$k_x = \frac{2\pi}{L} n_x, \quad n_x = 0, \pm 1, \pm 2 \dots$$

Similarly, for y  $k_y = \frac{2\pi}{L} n_y, \quad n_y = 0, \pm 1, \pm 2 \dots$

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

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

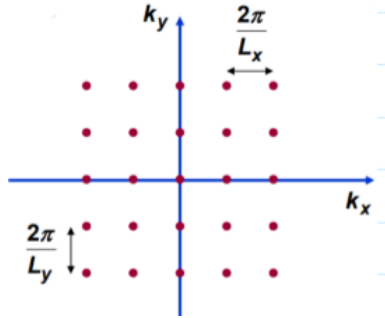


Figure 1: 2-D k space

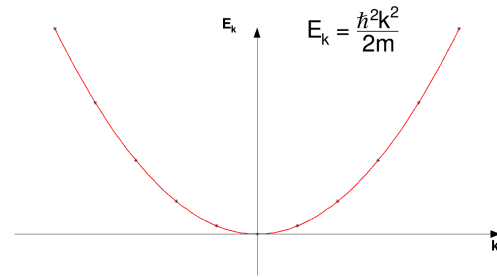


Figure 2:  $E_k = \frac{\hbar^2 k^2}{2m}$

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:

$$k_x = |k| \cos \varphi$$

$$k_y = |k| \sin \varphi$$

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

**Figure 2** shows this relation.

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.

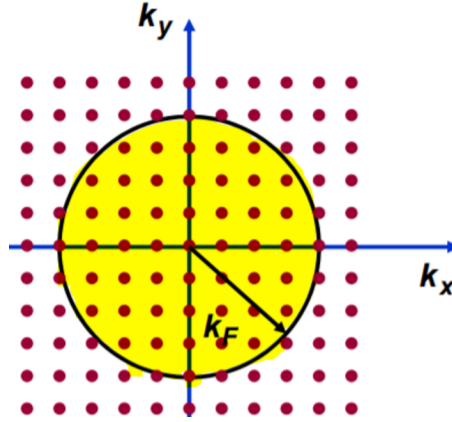


Figure 3: Fermi Surface in 2-D  $k$  space

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 :

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

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

**Answer:** Number of electrons is  $N$ :

$$\begin{aligned} N &= 2 \sum_{\vec{k}} \theta(k_F - |\vec{k}|) = 2 \iint_{|\vec{k}| < k_F} dn_x dn_y \\ &= 2 \iint \frac{L dk_x}{2\pi} \cdot \frac{L dk_y}{2\pi} = \frac{2A}{(2\pi)^2} \iint dk_x dk_y \\ &= \frac{2A}{(2\pi)^2} \int_0^{k_F} |k| d|k| \cdot \int_0^{2\pi} d\varphi = \frac{2A}{(2\pi)^2} \cdot \pi \cdot |k_F|^2 \\ &= \frac{A}{2\pi} |k_F|^2 \end{aligned}$$

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

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  $n = \frac{N}{V} = \frac{|k_F|^3}{3\pi^2}$

7. An important quantity is the density of states, or DOS :

$$N_n(E) = 2 \sum_{\vec{k}} \delta(E_{\vec{k}} - E)$$

Do the necessary integration, in the standard fashion, and show that the DOS is a constant  $N_n(E) = N_n$ . Polar coordinates should be helpful.

**Answer:**

$$\begin{aligned}
 N_n(E) &= 2 \sum_{\vec{k}} \delta(E_{\vec{k}} - E) \\
 &= 2 \iint dn_x dn_y \delta(E_k - E) \\
 &= 2 \left(\frac{L}{2\pi}\right)^2 \iint dk_x dk_y \delta(\dots) \\
 &= 2 \left(\frac{L}{2\pi}\right)^2 \int_0^\infty k dk \int_0^{2\pi} d\varphi \delta(\dots) = \frac{A}{\pi} \int_0^\infty k dk \delta(\dots) \\
 &= \frac{A}{\pi} \int_0^\infty k \frac{dk}{dE_k} dE_k \delta(E_k - E) \\
 &= \frac{A}{\pi} \cdot k \left(\frac{dk}{dE_k}\right)_{E_k=E}
 \end{aligned}$$

According to  $E_k = \frac{\hbar^2 k^2}{2m}$

We have  $\frac{dE_k}{dk} = \frac{\hbar^2}{m} \cdot k$

$$k \frac{dk}{dE_k} = \frac{m}{\hbar^2}$$

So  $N_n(E)$  is  $= \frac{Am}{\pi \hbar^2}$

And DOS is thus  $\frac{N_n(E)}{A} = \frac{m}{\pi \hbar^2} = cte.$

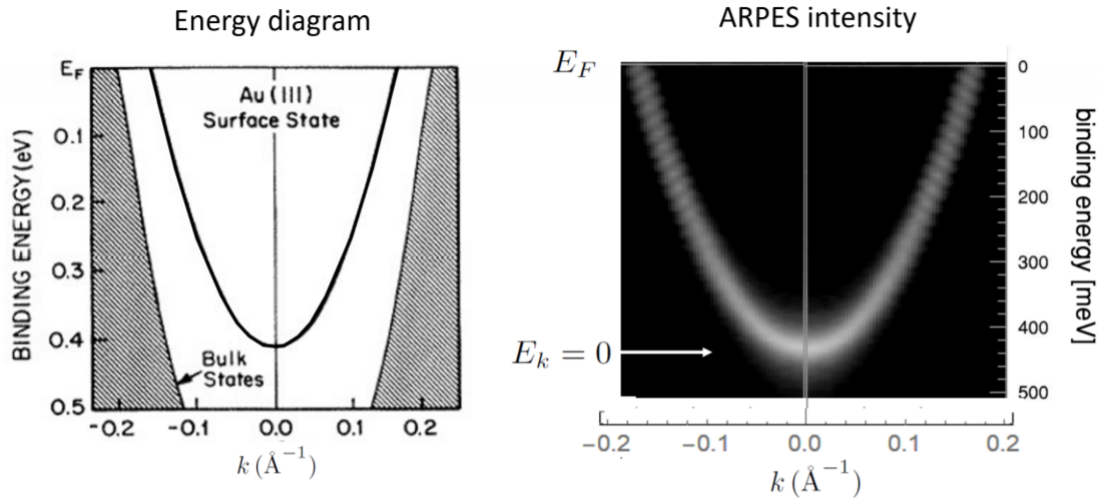


Figure 4: Au(111) ARPES spectrum

8. As shown in the figure above (right panel), the energy band  $E_k$  is directly visible in the ARPES intensity as a function of the parallel wave vector. From the experimental curve, please give an estimate of the Fermi wave-vector  $k_F$  and the Fermi energy  $E_F$ .

**Answer:** The  $k_F$  is around  $0.16 \text{ \AA}^{-1}$ , according to  $E_F = \frac{\hbar^2 k_F^2}{2m}$ ,  $E_F = 0.1 \text{ eV}$

9. Use your expression for the electron density  $n$  to estimate it using the experimental value for  $k_F$ . One decimal precision is enough and express  $n$  in both  $\text{m}^{-2}$  and  $\text{\AA}^{-2}$  units. If the distance between two gold atoms is  $\sim 3 \text{ \AA}$ , how many electrons are there per surface unit cell (the lattice is triangular) ?

**Answer:** The electron density is  $n = \frac{|k_F|^2}{2\pi}$ ,  $k_F = 0.16 \text{ \AA}^{-1}$ , so  $n = 4.1 \times 10^{-3} \text{ \AA}^{-2} = 4.1 \times 10^{17} \text{ m}^{-2}$ . The triangular area is  $\frac{\sqrt{3}}{4} r^2 = \frac{9\sqrt{3}}{4} \text{ \AA}^{-2}$ , number of electrons in this unit cell is 0.016.

10. Such an electron gas could indeed be superconducting, but the weak coupling with phonons and low Fermi-level DOS are not favorable. However, suppose that 0.1% of the electrons could become Cooper pairs in the superconducting state. Using the present study, estimate the predicted energy gap in a BCS model and the corresponding critical temperature  $T_c$ . (We recall that the number of Cooper pairs is :  $N_n(E_F)\Delta_0/2$ .)

**Answer:** Number of Cooper pairs is  $\frac{N_n(E_F)\Delta_0}{2}$ , so we have:

$$\frac{N_n(E_F)\Delta_0}{2} = 0.016 \times 0.1\%$$

$$\Delta_0 = 7.87 \times 10^{-4} \text{ eV}$$

$$1 \text{ eV} \rightarrow 10^4 \text{ K}$$

So critical temperature is  $T_c = 7.87 \times 10^{-4} \text{ eV} \approx 7.87 \text{ K}$

## II. The BCS effective Hamiltonian.

11. Starting from  $\tilde{H}_{eff} = \begin{pmatrix} \varepsilon_k & -\Delta_k \\ -\Delta_k^* & -\varepsilon_k \end{pmatrix}$  find the two eigenvalues  $E_k^+, E_k^-$  (Let us consider only  $\Delta_k$  is real.)

**Answer:** In the BCS 'mean-field' approximation, we showed that the electron/hole operators satisfy the simultaneous equations :

$$\begin{aligned} i\hbar \frac{d}{dt} (a_{k\uparrow}) &= \varepsilon_k a_{k\uparrow} - \Delta_k a_{-k\downarrow}^\dagger \\ i\hbar \frac{d}{dt} (a_{-k\downarrow}^\dagger) &= -\varepsilon_k a_{-k\downarrow}^\dagger - \Delta_k^* a_{k\uparrow} \end{aligned}$$

We can rewrite it into matrix form or say **Nambu Formalism**:

$$i\hbar \frac{d}{dt} \begin{pmatrix} a_{k\uparrow} \\ a_{-k\downarrow}^\dagger \end{pmatrix} = \begin{pmatrix} \varepsilon_k & -\Delta_k \\ -\Delta_k^* & -\varepsilon_k \end{pmatrix} \begin{pmatrix} a_{k\uparrow} \\ a_{-k\downarrow}^\dagger \end{pmatrix}$$

In order to diagonalize the matrix  $\begin{pmatrix} \varepsilon_k & -\Delta_k \\ -\Delta_k^* & -\varepsilon_k \end{pmatrix}$  and make it become the eigenfunction:

$$i\hbar \frac{d\tilde{\psi}}{dt} = \tilde{H}_{eff} \tilde{\psi}$$

We introduce the **Bogoliubov Transformation**, by which we can transfer the eigenfunction to a quasiparticle's eigenfunction with eigenvector  $\begin{pmatrix} \gamma^+ \\ \gamma^- \end{pmatrix}$  and eigenvalues  $\tilde{H}_{eff}$ .

First, we calculate the eigenvalues(energy):

$$(E_k - \tilde{H}_{eff}) \begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} E_k - \varepsilon_k & +\Delta_k \\ +\Delta_k^* & E_k + \varepsilon_k \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix} = 0$$

It gives an obvious solution:  $E_k = \sqrt{\Delta_k^2 + \varepsilon_k^2}$ , so

$$E_k^\pm = \pm \sqrt{\Delta_k^2 + \varepsilon_k^2}$$

12. Show a plot of the quasiparticle energy  $E_k^+$  as a function of  $\varepsilon_k$  and compare it to the case of 'normal' electrons.

**Answer:** As shown in **Figure 5**, for quasiparticles, it's  $E_k$  is a hyperbola function to  $\varepsilon_k$ , while for normal electrons,  $\Delta_k$  is 0, so  $E_k$  has linear relation with  $\varepsilon_k$ .

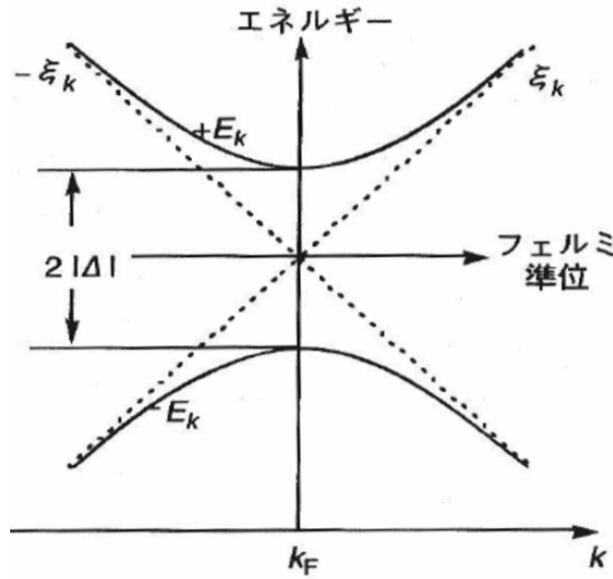


Figure 5: Relation between  $E_k$  and  $\varepsilon_k$  (Solid line-quasiparticles, Dash line-normal electrons)

13. We wish to derive the corresponding (2-dimensional) eigenvectors  $U^+$  and  $U^-$ . In the first case, we can write :

$$U^+ = \begin{pmatrix} u_k \\ v_k \end{pmatrix}$$

After some algebra, you should be able to find the standard amplitude functions :  $u_k$  and  $v_k$ , having the property  $u_k^2 + v_k^2 = 1$ .

**Answer:** We know  $\tilde{\Lambda}$  can diagonalize  $H_{eff}$

$$H_{eff} \xrightarrow{\tilde{\Lambda}} \begin{pmatrix} +\sqrt{\varepsilon_k^2 + \Delta_k^2} & 0 \\ 0 & -\sqrt{\Delta_k^2 + \varepsilon_k^2} \end{pmatrix}$$

$\tilde{\Lambda}$  can be generated by two eigenvectors, to get them, we employ again the eigenfunction:

$$\begin{pmatrix} E_k - \varepsilon_k & \Delta_k \\ \Delta_k^* & E_k + \varepsilon_k \end{pmatrix} \begin{pmatrix} u_k \\ v_k \end{pmatrix} = 0$$

$$\begin{aligned} (E_k - \varepsilon_k) u_k + \Delta_k v_k &= 0 \\ \Delta_k^* u_k + (E_k + \varepsilon_k) v_k &= 0 \\ u_k^2 + v_k^2 &= 1 \end{aligned}$$

Then we can get  $U^+$ : First, we have:

$$\frac{v_k}{u_k} = \frac{\sqrt{\varepsilon_k^2 + |\Delta_k|^2} - \varepsilon_k}{-\Delta_k^*}$$

Then, with  $u_k^2 + v_k^2 = 1$ ,

$$|u_k|^2 = \frac{1}{1 + \left| \frac{v_k}{u_k} \right|^2} = \frac{1}{2} \frac{|\Delta_k|^2}{\varepsilon_k^2 + |\Delta_k|^2 - \varepsilon_k \sqrt{\varepsilon_k^2 + |\Delta_k|^2}}$$

$$|u_k|^2 = \frac{1}{2} \frac{|\Delta_k|^2 \left( \sqrt{\varepsilon_k^2 + |\Delta_k|^2} + \varepsilon_k \right)}{(\sqrt{\varepsilon_k^2 + |\Delta_k|^2}) (\varepsilon_k^2 + |\Delta_k|^2 - \varepsilon_k^2)}$$

$$|u_k|^2 = \frac{1}{2} \left( 1 + \frac{\varepsilon_k}{\sqrt{\varepsilon_k^2 + |\Delta_k|^2}} \right) = \frac{1}{2} \left( 1 + \frac{\varepsilon_k}{E_k} \right)$$

$$|v_k|^2 = \frac{1}{2} \left( 1 - \frac{\varepsilon_k}{\sqrt{\varepsilon_k^2 + |\Delta_k|^2}} \right) = \frac{1}{2} \left( 1 - \frac{\varepsilon_k}{E_k} \right)$$

These are the amplitude functions.

14. Express the  $2 \times 2$  transformation matrix  $\tilde{\Lambda} = (U^+, U^-)$

**Answer:** For another eigenvalue  $E^-$ , the eigenvector is  $\begin{pmatrix} -v_k \\ u_k \end{pmatrix}$  So the transform matrix  $\tilde{\Lambda} = (U^+, U^-)$  is:

$$\tilde{\Lambda} = \begin{pmatrix} u_k & -v_k \\ v_k & u_k \end{pmatrix}$$

15. Using  $\tilde{\Lambda}$  find the new QP operators  $\gamma_k^+$  and  $\gamma_k^-$  in terms of  $a_{k\uparrow}$  and  $a_{-k\downarrow}^\dagger$ . Please give a physical interpretation of the quantities:  $\gamma_k^\pm$ ,  $u_k$ , and  $v_k$

**Answer:**

$$\tilde{\gamma}_k = \begin{pmatrix} \gamma_k^+ \\ \gamma_k^- \end{pmatrix} = \Lambda \tilde{a}_k = \Lambda \begin{pmatrix} a_{k,\uparrow} \\ a_{-k,\downarrow}^* \end{pmatrix} = \begin{pmatrix} u_k & -v_k \\ v_k & u_k \end{pmatrix} \begin{pmatrix} a_{k,\uparrow} \\ a_{-k,\downarrow}^* \end{pmatrix}$$

So,

$$\gamma_k^+ = u_k a_{k,\uparrow} - v_k a_{-k,\downarrow}^*$$

$$\gamma_k^- = v_k a_{k,\uparrow} + u_k a_{-k,\downarrow}^*$$

The physical meaning of  $\gamma_k^+$  and  $\gamma_k^-$  is the creation and annihilation operators of quasiparticles,  $a_{-k,\downarrow}^*$  and  $a_{k,\uparrow}$  are creation operators of electrons and holes.

From previous result describing the behavior of  $u_k$  and  $v_k$ , we have that as  $\Delta_k \rightarrow 0, |u_k|^2 \rightarrow 1$  for  $\varepsilon_k > 0$  and  $|u_k|^2 \rightarrow 0$  for  $\varepsilon_k < 0$  whereas  $|v_k|^2 \rightarrow 1$  for  $\varepsilon_k < 0$  and  $|v_k|^2 \rightarrow 0$  for  $\varepsilon_k > 0$ . So  $u_k^2$  and  $v_k^2$  correspond to possibility to find holes and electrons.



At the superconducting state, a quasiparticle is a superposition of both an electron and a hole state. And  $u_k$  corresponds to the amplitude of hole and  $v_k$  the amplitude of electron.

### Backup

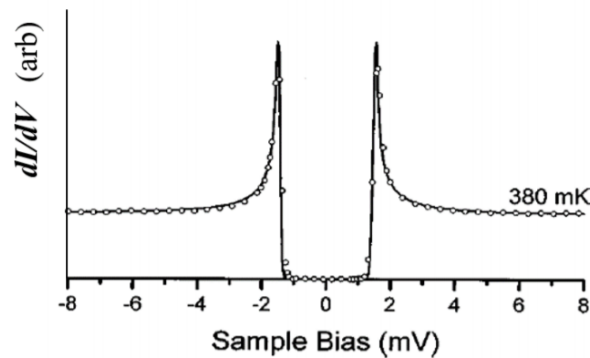
In other text books, I found they call  $\gamma_{k\sigma}^\dagger$  Bogoliubons and correspond to the excitation of quasiparticle.

In that book, it also mentioned:

**At the normal state, creating a quasiparticle corresponds to creating an electron for energies above the Fermi level and creating a hole (destroying an electron) of opposite momentum and spin for energies below the Fermi level.**

But from my equations, this process seemed to corresponds to  $\gamma^-$ , so I am a little confused.

16. The figure below shows the  $dI/dV$  measurement as a function of the voltage  $V$  for a niobium-vacuum-gold *tunneling junction*. The critical temperature of niobium is known to be 9.3 Kelvin. Does the theory (black line) agree well with the experiment (circular dots)? Please explain the key points in a few sentences.



Pan, Hudson and Davis, APL **73** (1998)

Figure 6:  $dI/dV$  of Nb tip-Au

**Answer:** Yes, they agree very well. And it indicates a superconducting quasiparticle DOS at the Nb-tip end. So we can see the gap clearly.