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,

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

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

$$\Downarrow$$

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

$$\Downarrow$$

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

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

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 $\left(\frac{2\pi}{L}\right)^2$
Of course, if we consider spin, then we have **two** states in such box.

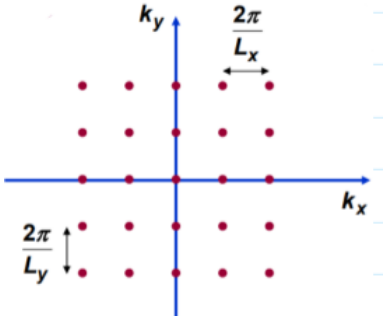

Figure 1: 2-D k space

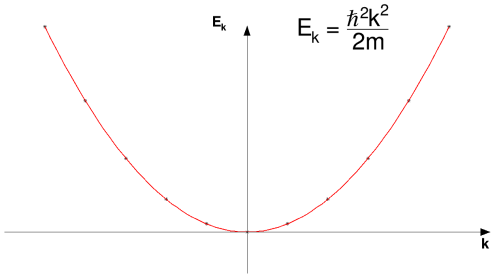

Figure 2: $E_k = \frac{\hbar^2 k^2}{2m}$

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:

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

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.

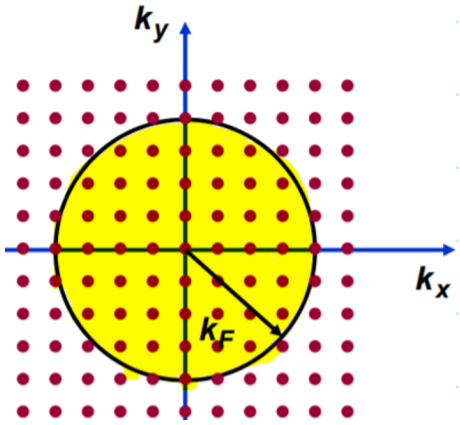

Figure 3: Fermi Surface in 2-D k space

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 :

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

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

Answer: Number of electrons is N:

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

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

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

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

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:

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

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

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

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

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

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

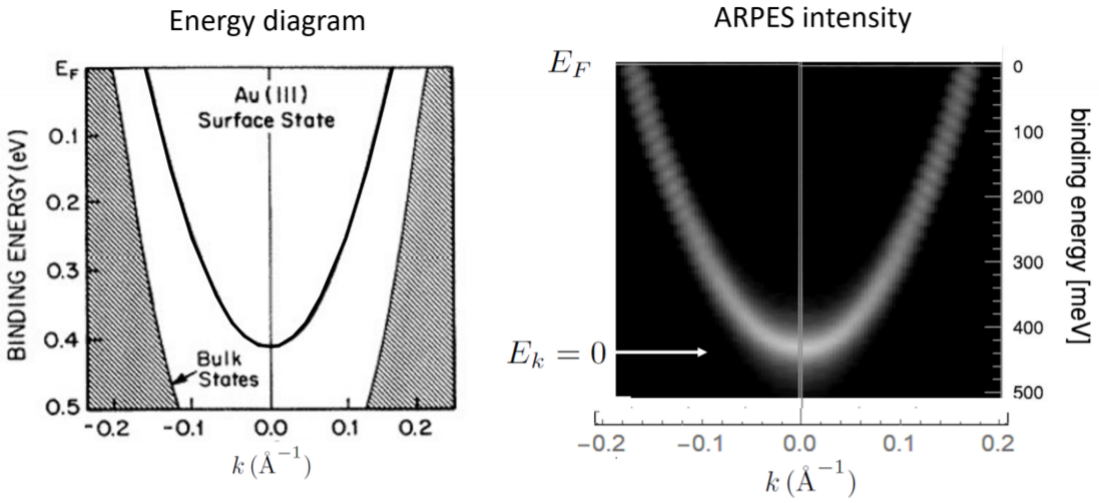

Figure 4: Au(111) ARPES spectrum

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 0.16Å^{-1} , according to $E_F = \frac{\hbar^2 k_F^2}{2m}$, $E_F = 0.1eV$

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 m^{-2} and Å^{-2} units. If the distance between two gold atoms is ~ 3Å, how many electrons are there per surface unit cell (the lattice is triangular) ?

Answer: The electron density is $n = \frac{|k_F|^2}{2\pi}$, $k_F = 0.16\text{Å}^{-1}$, so $n = 4.1 \times 10^{-3}\text{Å}^{-2} = 4.1 \times 10^{17} m^{-2}$
The triangular area is $\frac{\sqrt{3}}{4} r^2 = \frac{9\sqrt{3}}{4}\text{Å}^{-2}$, 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:

$$\frac{N_n(E_F)\Delta_0}{2} = 0.016 \times 0.1\%$$
$$\Delta_0 = 7.87 \times 10^{-4} eV$$
$$1eV \approx 10^4 K$$
So citical temperature is $T_c = 7.87 \times 10^{-4} eV \approx 7.87K$

II. The BCS effective Hamiltonian.

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

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

$$i\hbar \frac{d}{dt}\left(a_{k\uparrow}\right) = \epsilon_k a_{k\uparrow} - \Delta_k a^\dagger_{-k\downarrow}$$
$$i\hbar \frac{d}{dt}\left(a^\dagger_{-k\downarrow}\right) = -\epsilon_k a^\dagger_{-k\downarrow} - \Delta_k^* a_{k\uparrow}$$

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

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

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

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

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 eignvalues(energy):

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

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

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

12. Show a plot of the quasiparticle energy E_k^+ as a function of ϵ_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 ϵ_k, while for normal electrons, Δ_k is 0, so E_k has linear relation with ϵ_k.

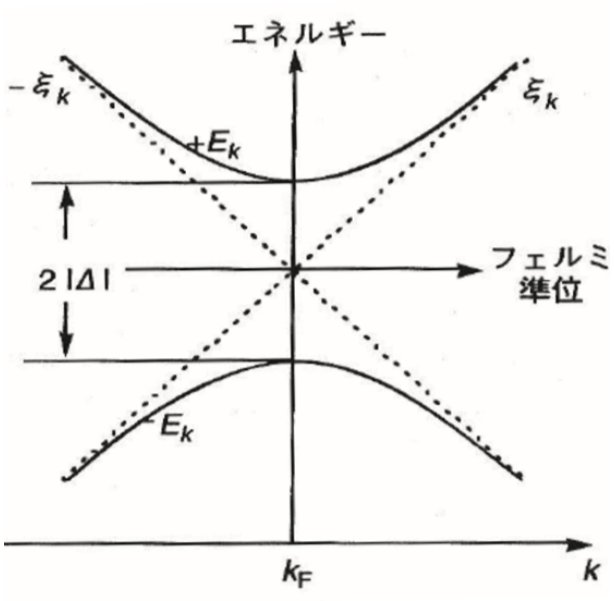

Figure 5: Relation between E_k and ϵ_k(Solid line-quasiparticles,Dash line-normal electrons)

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}

$$H_{eff} \overset{\tilde{\Lambda}}{\Rightarrow} \begin{pmatrix} +\sqrt{\epsilon_k^2 + \Delta_k^2} & 0 \\ 0 & -\sqrt{\Delta_k^2 + \epsilon_k^2} \end{pmatrix}$$

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

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

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

$$\frac{v_{\mathbf{k}}}{u_{\mathbf{k}}} = \frac{\sqrt{\epsilon_{\mathbf{k}}^2 + |\Delta_{\mathbf{k}}|^2} - \epsilon_{\mathbf{k}}}{-\Delta_{\mathbf{k}}^*}$$

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

$$|u_{\mathbf{k}}|^2 = \frac{1}{1 + \left|\frac{v_{\mathbf{k}}}{u_{\mathbf{k}}}\right|^2} = \frac{1}{2}\frac{|\Delta_{\mathbf{k}}|^2}{\epsilon_{\mathbf{k}}^2 + |\Delta_{\mathbf{k}}|^2 - \epsilon_{\mathbf{k}}\sqrt{\epsilon_{\mathbf{k}}^2 + |\Delta_{\mathbf{k}}|^2}}$$

$$|u_{\mathbf{k}}|^2 = \frac{1}{2}\frac{|\Delta_{\mathbf{k}}|^2\left(\sqrt{\epsilon_{\mathbf{k}}^2 + |\Delta_{\mathbf{k}}|^2} + \epsilon_{\mathbf{k}}\right)}{(\sqrt{\epsilon_{\mathbf{k}}^2 + |\Delta_{\mathbf{k}}|^2})\left(\epsilon_{\mathbf{k}}^2 + |\Delta_{\mathbf{k}}|^2 - \epsilon_{\mathbf{k}}^2\right)}$$

$$|u_{\mathbf{k}}|^2 = \frac{1}{2}\left(1 + \frac{\epsilon_{\mathbf{k}}}{\sqrt{\epsilon_{\mathbf{k}}^2 + |\Delta_{\mathbf{k}}|^2}}\right) = \frac{1}{2}\left(1 + \frac{\epsilon_{\mathbf{k}}}{E_k}\right)$$

$$|v_{\mathbf{k}}|^2 = \frac{1}{2}\left(1 - \frac{\epsilon_{\mathbf{k}}}{\sqrt{\epsilon_{\mathbf{k}}^2 + |\Delta_{\mathbf{k}}|^2}}\right) = \frac{1}{2}\left(1 - \frac{\epsilon_{\mathbf{k}}}{E_k}\right)$$

These are the amplitude functions.

14. Express the 2×2 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 γ_k^+ and γ_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 physicsl meaning of γ_k^+ and γ_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 $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$, we have that as $\Delta_{\mathbf{k}} \to 0$,$|u_{\mathbf{k}}|^2 \to 1$ for $\epsilon_{\mathbf{k}} > 0$ and $|u_{\mathbf{k}}|^2 \to 0$ for $\epsilon_{\mathbf{k}} < 0$ whereas $|v_{\mathbf{k}}|^2 \to 1$ for $\epsilon_{\mathbf{k}} < 0$ and $|v_{\mathbf{k}}|^2 \to 0$ for $\epsilon_{\mathbf{k}} > 0$. So $u_{\mathbf{k}}^2$ and $v_{\mathbf{k}}^2$ 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 $\gamma^{\dagger}_{\mathbf{k}\sigma}$ 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 γ^{-} , 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.

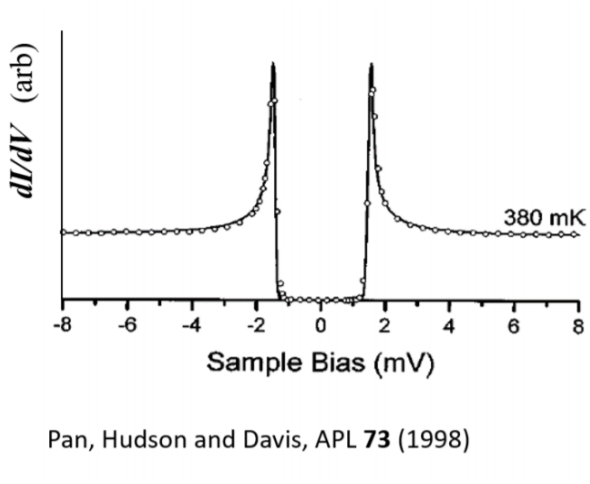

Figure 6: dI/dV of Nb tip-Au

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.