ECE 5390 / MSE 5472, Fall Semester 2017

Quantum Transport in Electron Devices and Novel Materials

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Assignment 4, Solutions

Problem 4.1: Survey of Superconductivity

Problem 4.1) Survey of Superconductivity

Create a well-thought out table of the experimental status of various superconducting materials and their transport and related properties such as critical parameters T_c, H_c, J_c, gaps Δ, London penetration depths λ_L, material stability, and other parameters you consider important. Include high-T_c superconductors, and superconductors that are semiconductors under normal conditions. Indicate in the table which ones are used for industrial applications, and for what.

Solution: [By Ian Briggs and Sayak Ghosh, 2017]

Material	Tc (K)	Hc (T)	electron density (1/m^3)	Debye Temperature (K)	Fermi Energy (eV)	Lambda_L (Angstroms)	coherence length (nm)	Delta (meV)
Al	1.2	0.01	1.81E+29	433	11.7	88	50	0.1
Diamond: B	11.4	4						0.98
Ga	1.083	0.0058	1.54E+29	325	10.4	96	64	0.09
Nb	9.26	0.82	5.56E+28	276	5.32	159	54	0.8
In	3.4	0.03	1.15E+29	112	8.63	111	168	0.29
C60K3	19.8	0.013						1.71
Nb3Ge	23	38			vf1 = 2.2e7 cm/s		35-50 Angstroms	1.98
BKBO	31	32			vf2 = 3.0e7 cm/s		35-50 Angstroms	2.67
MgB2	39	39			vf3 = 4.8e7 cm/s		35-50 Angstroms	3.36
PbMo6S8	15	60						1.29
LaMo6S8	7	44.5						0.6
SnMo6S8	12	36						1.03
Mo	0.92	0.0096		423				0.079
Hg	4	0.04	8.65E+28	72	7.13	128	238	0.34

	Superconductor	Tc(K)	Hc(T)	Delta(eV)	lambda(nm)
Element	mercury	4.2	0.041	7.17E-04	100
	tin	3.7	0.037	5.74E-04	50
	lead	7.2	0.08	1.23E-03	30.5
	niobium	9.2	0.82	1.45E-03	45
Binary Compounds	NbTi	9.2	15	1.39E-03	
	V3Si	17.1	20	2.58E-03	
	Nb3Sn	18	28	2.72E-03	
	MgB2	39	74	5.89E-03	
Heavy fermion	CeCu2Si2	0.7	2.5	Not isotropic gap	
	UPt3	0.55	0.3		
	CeCoIn5	2.4	0.5		
	PuCoGa5	18.5		6.00E-03	
Cuprates	LSCO	39	82	Not isotropic gap	
	YBCO	92	150		
	BiSrCaCuO(2212)	110	200		
	HgBaCaCuO(1223)	134			

Problem 4.2: Current Transport in Josephson Junctions

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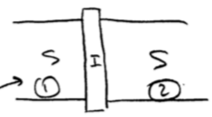
We have discussed how the Ginzburg-Landau theory explains superconductivity by introducing the macroscopic wavefunction $\Psi(r) = \sqrt{n(r)}e^{i\theta(r)}$, and in one masterstroke explains all the hallmarks of transport and related properties of superconductors such as persistent currents, the Meissner effect and London penetration depths, flux quantization, etc. This theory is also central to understanding most superconducting quantum devices, the Josephson junction being a prime example.
In class I outlined how to understand the rather remarkable current-voltage characteristics of a superconductor/insulator/superconductor junction in which Cooper pairs can tunnel from one superconductor to the other, leading to the flow of a ac Josephson current

$$I = I_0 \sin(\frac{2eV}{\hbar}t + \alpha), \tag{1}$$

where all terms have their usual meanings. Using the Landau-Ginzburg macroscopic wavefunctions $\Psi_1 = \sqrt{n}_1 e^{i\theta_1}$ and $\Psi_2 = \sqrt{n}_2 e^{i\theta_2}$ and using Schrodinger equation allowing for tunneling from one superconductor to the other, show that the current given by Equation 1. Assume $n_1 \approx n_2$. Discuss what is rather remarkable about the transport in this superconducting device, and show that $V \approx 1$ mV across the tunnel diode leads to an oscillation frequency of ~ 3 THz. Explain how such junctions are used in SQUID magnetometers.

Solution: [By Andrei Isichecko, 2017]

Problem 2 Current Transport in Josephson Junction



$$\Longrightarrow I(t) = I_0 \sin\left(\frac{2eV}{\hbar}t + \alpha\right)$$

$$\Psi_1 = \sqrt{n_1}\, e^{i\theta_1} \qquad \Psi_2 = \sqrt{n_2}\, e^{i\theta_2} \qquad \text{where } n_1 \simeq n_2$$

coupling coefficient

$$\begin{cases} i\hbar \dfrac{\partial \Psi_1}{\partial t} = E_1 \Psi_1 + a \Psi_2 \\ i\hbar \dfrac{\partial \Psi_2}{\partial t} = E_2 \Psi_2 + a \Psi_1 \end{cases}$$

$$\begin{cases} i\hbar \dfrac{\partial}{\partial t} \sqrt{n_1} e^{i\theta_1} = E_1 \sqrt{n_1} e^{i\theta_1} + a\sqrt{n_2}\, e^{i\theta_2} \\ i\hbar \dfrac{\partial}{\partial t} \sqrt{n_2} e^{i\theta_2} = E_2 \sqrt{n_2} e^{i\theta_2} + a\sqrt{n_1}\, e^{i\theta_1} \end{cases}$$

$$\begin{cases} \dfrac{i\hbar}{2} \dot{n}_1 e^{i\theta_1} - \hbar n_1 \dot{\theta}_1 e^{i\theta_1} = E_1 n_1 e^{i\theta_1} + a\sqrt{n_1 n_2}\, e^{i\theta_2} \\ \dfrac{i\hbar}{2} \dot{n}_2 e^{i\theta_2} - \hbar n_2 \dot{\theta}_2 e^{i\theta_2} = E_2 n_2 e^{i\theta_2} + a\sqrt{n_1 n_2}\, e^{i\theta_1} \end{cases}$$

$$E_2 - E_1 = eV \qquad \text{let } E_1 = -\frac{eV}{2} \qquad E_2 = \frac{eV}{2}$$

Seperate real and imaginary parts.

$$\frac{\hbar \dot{n}_1}{2}\left(i\cos\theta_1 - \sin\theta_1\right) - \hbar n_1 \dot{\theta}_1 (\cos\theta_1 + i\sin\theta_1) = E_1 n_1 (\cos\theta_1 + i\sin\theta_1) + a\sqrt{n_1 n_2}(\cos\theta_2 + i\sin\theta_2)$$

$$\begin{cases} \text{im: } \dfrac{\hbar \dot{n}_1}{2}\cos\theta_1 - \hbar n_1 \dot{\theta}_1 \sin\theta_1 = n_1 E_1 \sin\theta_1 + a\sqrt{n_1 n_2}\sin\theta_2 \\ \text{real: } -\dfrac{\hbar \dot{n}_1}{2}\sin\theta_1 - \hbar n_1 \dot{\theta}_1 \cos\theta_1 = n_1 E_1 \cos\theta_1 + a\sqrt{n_1 n_2}\cos\theta_2 \end{cases}$$

$$\begin{cases} \text{im: } \dfrac{\hbar \dot{n}_2}{2}\cos\theta_2 - \hbar n_2 \dot{\theta}_2 \sin\theta_2 = n_2 E_2 \sin\theta_2 + a\sqrt{n_1 n_2}\sin\theta_1 \\ \text{real: } -\dfrac{\hbar \dot{n}_2}{2}\sin\theta_2 - \hbar n_2 \dot{\theta}_2 \cos\theta_2 = n_2 E_2 \cos\theta_2 + a\sqrt{n_1 n_2}\cos\theta_1 \end{cases}$$

4 equations recording real and imaginary parts in each case.

eliminate 1 equation and coupling coefficient a

$$\frac{\hbar \dot{n}_2}{2}\cos\theta_1\cos\theta_2 - \hbar n_2 \dot{\theta}_2 \cos\theta_1 \sin\theta_2 = \frac{n_2 eV}{2}\sin\theta_2\cos\theta_1 + a\sqrt{n_1 n_2}\sin\theta_1\cos\theta_1$$

$$- \quad -\frac{\hbar \dot{n}_2}{2}\sin\theta_1\sin\theta_2 - \hbar n_2 \dot{\theta}_2 \sin\theta_1\cos\theta_2 = \frac{n_2 eV}{2}\sin\theta_1\cos\theta_2 + a\sqrt{n_1 n_2}\cos\theta_1\sin\theta_1$$

$$\frac{\hbar \dot{n}_2}{2}\left(\cos\theta_1\cos\theta_2 + \sin\theta_1\sin\theta_2\right) - \hbar n_2 \dot{\theta}_2 \left(\cos\theta_1\sin\theta_2 - \sin\theta_1\cos\theta_2\right) = \frac{n_2 eV}{2}\left(\sin\theta_2\cos\theta_1 - \sin\theta_1\cos\theta_2\right)$$

$$\rightarrow \frac{\hbar \dot{n}_2}{2}\cos\delta = \left(\frac{n_2 eV}{2} + \hbar n_2 \dot{\theta}_2\right)\sin\delta \qquad \text{where } \delta \equiv \theta_2 - \theta_1$$

similarly, $$\frac{\hbar \dot{n}_1}{2}\cos(\delta) = \left(\frac{\hbar n_1 eV}{2} - \hbar n_1 \dot{\theta}_1\right)\sin\delta$$

This means that:

$$\frac{dn_2}{dt} = n_2\left(\frac{eV}{\hbar} + 2\dot{\theta}_2\right)\tan\delta$$

$$\frac{dn_1}{dt} = n_1\left(\frac{eV}{\hbar} - 2\dot{\theta}_1\right)\tan\delta$$

And because $\dot{n}_1 = -\dot{n}_2$, $n_1 \simeq n_2$, adding eqns $\Rightarrow 0 = n\left(\frac{2eV}{\hbar} + 2(\dot{\theta}_2 - \dot{\theta}_1)\right)\tan\delta$

$$\hookrightarrow \boxed{\dot{\theta}_2 - \dot{\theta}_1 = \frac{eV}{\hbar}}$$

we can also show that

$$\frac{\partial n_1}{\partial t} = \frac{2}{\hbar} a \sqrt{n_1 n_2}\sin\delta \quad \text{and} \quad \frac{\partial n_2}{\partial t} = \frac{-2}{\hbar} a \sqrt{n_1 n_2}\sin\delta \;\Big\}\; \dot{n}_1 = -\dot{n}_2$$

$$\frac{\partial \theta_1}{\partial t} = -\frac{a}{\hbar}\sqrt{\frac{n_2}{n_1}}\cos\delta - \frac{eV}{2\hbar} \quad \text{and} \quad \frac{\partial \theta_2}{\partial t} = -\frac{a}{\hbar}\sqrt{\frac{n_2}{n_1}}\cos\delta + \frac{eV}{2\hbar}$$

$\partial n/\partial t \rightarrow$ $$I = \underbrace{\frac{2a}{\hbar}\sqrt{n_1 n_2}}_{I_0}\sin\delta$$

$\delta(t) = \int \dot{\delta}(t)\,dt$

$\downarrow$ const

$\delta(t) = \dot{\delta} t + \alpha \longleftarrow \dot{\delta} = \dot{\theta}_2 - \dot{\theta}_1 = \frac{eV}{\hbar} \rightarrow \frac{2eV}{\hbar}$ $\quad e \rightarrow 2e$ for a pair

$$\therefore \boxed{I = I_0 \sin\left(\frac{2eV}{\hbar}t + \alpha\right)}$$

$\alpha \rightarrow$ phase factor

Transport in the device is remarkable because there is an AC current when a DC voltage is applied!

for $V = 1\,mV$, $\omega = \frac{2eV}{\hbar}$ //N $= 3.09\times10^{12}\,Hz = \boxed{3\,THz}$

Such junctions are used in SQUID magnetometers, which have 2 Josephson Junction in parallel that will detect a voltage variation for a changing magnetic flux in loop. Because the magnetic flux quantum is $\sim 10^{-15}\,T\cdot m^2$, this device is very sensitive.

Problem 4.3: Cooper pairs in Superconductors

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In this problem, we expose the limitations of perturbation theory in quantum mechanics. The reason why it took nearly half a century from the experimental discovery of superconductivity to the development of a theory for it is because its physics cannot be obtained from perturbation theory. One has to solve the Hamiltonian problem more or less *exactly* - even if for a simplified toy model that captures the essential physics. Now Bardeen, Cooper, and Schrieffer (BCS) constructed such a theory. We first solve the toy model that Cooper did to unlock the mystery.

(a) Working in the Fourier (k-)space, show that for an electron of mass m moving in 1D with an attractive Dirac-delta potential $V(x) = -\alpha\delta(x)$, there is *exactly* one bound state, no matter how small the strength α. Show that this bound-state energy is $E_0 = -\frac{m\alpha^2}{2\hbar^2}$.

(b) Following (a), set up the same problem for a $D-$dimensional Dirac-delta attractive potential for an electron moving in $D-$dimensions. Show why a naive search for bound states leads to divergent $k-$space integrals for $D > 1$. Fact: theorists just *love* such divergences!

(c) Tame the *ultraviolet divergence* as $k \to \infty$ by imposing an *ultraviolet cutoff* of $k_{max} = \frac{1}{a}$. This is a fancy way of saying that we will set a minimum floor on the wavelengths permitted for electrons. Find the required condition for bound states in $D-$dimensions with this UV cutoff.

(d) Now a great many profound physics discoveries have resulted from studying the long-wavelength, or the *infrared divergences*. This happens when integrals blow up as $k \to 0$, or electron wavelengths become very long. Show that for a *vanishingly weak* Delta-function $\alpha \to 0$, there cannot be a bound state for $D \geq 3$.

(e) Show that for $D = 2$, there is a bound state of energy $E_0 = -\frac{\hbar^2}{ma^2(e^{\frac{2\pi\hbar^2}{m\alpha}}-1)} \approx -\frac{\hbar^2}{ma^2}e^{-\frac{2\pi\hbar^2}{m\alpha}}$ for a vanishingly small attractive Dirac-delta potential as $\alpha \to 0$. Explain why this result is unattainable from perturbation theory.

(f) Now make the connection of this toy problem to the Cooper pair[1] problem we have discussed in class: two electrons of opposite momenta and opposite spins at the Fermi energy surface E_F of a metal bound by phonons of energy up to $\hbar\omega_D$ via a vanishingly weak pairing potential $-V_0$. Show how the pairing causes the 2-electron energy to reduce from $2E_F \to 2E_F - \Delta$, where $\Delta = (2\hbar\omega_D)e^{-\frac{2}{N_0 V_0}}$, where N_0 is the DOS at the Fermi energy. Discuss why the gap is small, and why it cannot be obtained from perturbation theory.

Solution: [By Sam Bader, 2015]

a)

Start from Schrodinger equation

$$\left(\frac{\hat{p}^2}{2m} - \alpha\delta(x)\right)\psi(x) = E\psi(x)$$

Fourier transform. The only non-trivial term to Fourier transform is the δ term. The transform of $\delta(x)\psi(x)$ is the convolution of the transforms of the factors. Since $\delta(x)$ transforms to a unity, this convolution is just an integral of the wavefunction in k-space:

$$\frac{\hbar^2 k^2}{2m}\psi(k) - \alpha\int\frac{dk'}{2\pi}\psi(k') = E\psi(k)$$

Rearranging

$$\psi(k) = \frac{\alpha \int \frac{dk'}{2\pi}\psi(k')}{\frac{\hbar^2 k^2}{2m} - E}$$

Integrate both sides by k

$$\int \frac{dk}{2\pi}\psi(k) = \int \frac{dk}{2\pi}\frac{\alpha}{\frac{\hbar^2 k^2}{2m} - E}\int \frac{dk'}{2\pi}\psi(k')$$

Cancel the integral factors

$$1 = \int \frac{dk}{2\pi}\frac{\alpha}{\frac{\hbar^2 k^2}{2m} - E}$$

Use $\int \frac{dx}{x^2 - E} = \frac{\pi}{\sqrt{-E}}$, valid for $E < 0$

$$1 = \frac{\sqrt{2m}\alpha\pi}{2\pi\hbar\sqrt{-E}}$$

So

$$E = -\frac{m\alpha^2}{2\hbar^2}$$

b)

Start as before

$$\left(\frac{\vec{p}^2}{2m} - \alpha\delta^D(\vec{x})\right)\psi(\vec{x}) = E\psi(\vec{x})$$

In Fourier space

$$\frac{\hbar^2 \vec{k}^2}{2m}\psi(\vec{k}) - \alpha \int \frac{d^D\vec{k}'}{(2\pi)^D}\psi(\vec{k}') = E\psi(\vec{k})$$

Rearranging

$$\psi(\vec{k}) = \frac{\alpha \int \frac{d^D\vec{k}'}{(2\pi)^D}\psi(\vec{k}')}{\frac{\hbar^2 k^2}{2m} - E}$$

Integrate both sides by k

$$\int \frac{d^D\vec{k}}{(2\pi)^D}\psi(\vec{k}) = \int \frac{d^D\vec{k}}{(2\pi)^D}\frac{\alpha}{\frac{\hbar^2 k^2}{2m} - E}\int \frac{d^D\vec{k}'}{(2\pi)^D}\psi(\vec{k}')$$

Cancel the integral factors

$$1 = \int \frac{d^D\vec{k}}{(2\pi)^D}\frac{\alpha}{\frac{\hbar^2 k^2}{2m} - E}$$

There are D powers of k on top and 2 powers of k in the denominator. So for $D \geq 2$, this integral diverges. (For instance, if $D = 2$, the Jacobian into spherical will contribute a k so the integrand goes as $k/k^2 = 1/k$ for large k, which gives a logarithmic divergence. Raise the dimensionality further, and the Jacobian gives more factors of k, producing stronger divergences.)

Taking advantage of the $(D-1)$-spherical symmetry of the integral, we switch to $(D-1)$-spherical coordinates. The only non-trivial integral is the radial direction, and the others combine to give a factor of the surface area of the $(D-1)$-sphere of radius k

$$1 = \frac{1}{2^{D-1}\pi^{D/2}\Gamma(D/2)}\int_0^{1/a} dk \frac{\alpha k^{D-1}}{\frac{\hbar^2 k^2}{2m} - E}$$

Non-dimensionalizing with $\kappa^2 = \frac{\hbar^2 k^2}{2m(-E)}$, $\kappa_m^2 = \frac{E_a}{(-E)}$ where $E_a = \frac{\hbar^2}{2ma^2}$

$$1 = \left[\frac{1}{2^{D-1}\pi^{D/2}\Gamma(D/2)}\right]\left[\alpha\left(\frac{2m}{\hbar^2}\right)^{D/2}(-E)^{D/2-1}\right]\left[\int_0^{\kappa_m} d\kappa \frac{\kappa^{D-1}}{\kappa^2+1}\right]$$

The case $D = 1$ was already explored (and can be reproduced here from the above expression). The case $D = 2$ will be discussed in (d), starting from here... So let me proceed to $D \geq 3$.

There are three physically sensible statements that I could imagine for a given dimension D.

- There is always a bound state (as we've shown for $D = 1$.)
- There is some threshold $\alpha = \alpha_D$ above which there is a bound state, below which there is none.

- There is no bound state, regardless of α. (As we'll see this statement doesn't apply to any D.)

If there is a threshold α_D, then we expect the bound state energy E to be vanishingly small as $\alpha \to \alpha_D^+$. So let's look for bound states with vanishingly small E to find this possible α threshold. For $E \ll \frac{\hbar^2}{2ma^2}$ (ie large κ_m) and $D \geq 3$, the integral will be dominated by the region where $\kappa \gg 1$, so we can ignore the 1 in the denomintor.

$$1 = \left[\frac{1}{2^{D-1}\pi^{D/2}\Gamma(D/2)}\right]\left[\alpha_D\left(\frac{2m}{\hbar^2}\right)^{D/2}(-E)^{D/2-1}\right]\left[\int_0^{\kappa_m} d\kappa\kappa^{D-3}\right]$$

$$1 = \left[\frac{1}{2^{D-1}\pi^{D/2}\Gamma(D/2)(D-2)}\right]\left[\alpha_D\left(\frac{2m}{\hbar^2}\right)^{D/2}(-E)^{D/2-1}\right]\left[\kappa_m^{D-2}\right]$$

$$1 = \left[\frac{1}{2^{D-1}\pi^{D/2}\Gamma(D/2)(D-2)}\right]\left[\frac{\alpha_D}{E_a a^D}\right]$$

So the threshold is

$$\alpha_D = \left[2^{D-1}\pi^{D/2}\Gamma(D/2)(D-2)\right]\left[E_a a^D\right]$$

The first factor is just a dimension-dependent number. The second factor is really the only combination of parameters we could make up with with right units. We've now found the α_D required for a bound state of vanishing energy in all dimensions $D \geq 3$, corresponding to the second of the three possibilities given above.

So, for $D \geq 3$, there is a bound state iff $\alpha > \alpha_D$, where α_D is given above. For $D = 1, 2$, there is always a bound state, as shown in part (a) and part (d).

c)

My argument in (b) shows that α must be above a certain value $\alpha_3 = \frac{\pi^2\hbar^2 a}{m}$ for there to be a bound state. So for a vanishingly weak δ potential in 3D, there is no bound state.

d)

Taking my expression from (b)

$$1 = \left[\frac{1}{2^{D-1}\pi^{D/2}\Gamma(D/2)}\right]\left[\alpha\left(\frac{2m}{\hbar^2}\right)^{D/2}(-E)^{D/2-1}\right]\left[\int_0^{\kappa_m} d\kappa\frac{\kappa^{D-1}}{\kappa^2+1}\right]$$

and plugging in $D = 2$

$$1 = \left[\frac{m\alpha}{2\pi\hbar^2}\right]\left[\int_0^{\kappa_m} d\kappa\frac{\kappa}{\kappa^2+1}\right]$$

This integral can be evaluated with the substitution $u = k^2 + 1$

$$1 = \left[\frac{m\alpha}{2\pi\hbar^2}\right]\left[\int_1^{\kappa_m^2+1}\frac{du}{u}\right]$$

$$1 = \left[\frac{m\alpha}{2\pi\hbar^2}\right]\left[\ln(\kappa_m^2+1)\right]$$

$$\kappa_m^2 = \exp\left\{\frac{2\pi\hbar^2}{m\alpha}\right\} - 1$$

$$E = -\frac{\hbar^2}{2ma^2}\frac{1}{\exp\left\{\frac{2\pi\hbar^2}{m\alpha}\right\} - 1}$$

This energy continues to be negative no matter how small α is, so we always have a bound state.

For small α, we can ignore the 1 in the denominator

$$E = -\frac{\hbar^2}{2ma^2}\exp\left\{-\frac{2\pi\hbar^2}{m\alpha}\right\}$$

Mathematically, we see that this energy goes as $e^{-1/\alpha}$ which is famously a non-analytic function at $\alpha = 0$. So perturbation theory, which is basically a Taylor expansion in α, can't possibly capture it.

e)

In translating between these problems we recognize our cut-off energy $E_a = \frac{\hbar^2}{2ma^2}$ should be the highest energies available to the the phonon-mediated interaction, $\hbar\omega_0$. And the delta magnitude α is the strength of the pairing interaction V_0. And then, re-examining the result from the previous problem, we see that the factor multiplying α inside the exponential is a free-electron density of states (divided by 2π), so we'll translate it to the density of states at the Fermi surface which (in 3D) goes as $\frac{8\pi m p_F}{h^3}$. Plugging in all that, we find

$$-\Delta = -\hbar\omega \; e^{-\frac{1}{N_0 V_0}}$$

with N_0 as given. Because we're basing our answer on the result in (d) that I already argued is beyond the reach of perturbation theory, this result is also non-perturbative.

Problem 4.4: The BCS Theory of Superconductivity

Problem 4.4) The BCS Theory of Superconductivity

(a) Show that an estimate of the critical current density that converts a superconductor of gap Δ to a normal metal is $J_c \approx 2en\frac{\Delta}{\hbar k_F}$, where n is the normal single-particle electron density, e the electron charge, and k_F is the Fermi wavevector. Show that for standard metals it evaluates to $J_c \sim 10^7$ A/cm^2. (You can imagine that the superconducting gap prevents scattering, till the single particle states have kinetic energies larger than the gap. Another way to picture this is to estimate the electron kinetic energy needed to break the Cooper pairs.)

In class we discussed the BCS Hamiltonian is

$$H_{BCS} = \sum_{\mathbf{k},\sigma} E_0(\mathbf{k}) c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} - V_0 \sum_{\mathbf{k},\mathbf{q}} c^\dagger_{\mathbf{q}\uparrow} c^\dagger_{-\mathbf{q}\downarrow} c_{-\mathbf{k}\downarrow} c_{\mathbf{k},\uparrow}, \quad (2)$$

and the BCS macroscopic wavefunction is

$$|\Psi_{BCS}\rangle = \prod_{\mathbf{k}} (u_{\mathbf{k}} + v_{\mathbf{k}} c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow})|0\rangle = \prod_{\mathbf{k}} (u_{\mathbf{k}} + v_{\mathbf{k}} b^\dagger_{\mathbf{k}})|0\rangle, \quad (3)$$

where $b^\dagger_{\mathbf{k}} = c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow}$ is the Cooper pair creation operator with the corresponding annihilation operator $b_{\mathbf{k}} = c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow}$. In Problem 2.2, you have seen that these operators composed of two fermionic operators look somewhat like Boson operators, but are not quite Bosonic. The terms $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ are unknown coefficients. For our purposes, assume them to be real (though this is not necessary).

(b) Show how normalization of the BCS macroscopic wavefunction $\langle \Psi_{BCS}|\Psi_{BCS}\rangle = 1$ followed by the minimization of the energy $\langle \Psi_{BCS}|H_{BCS}|\Psi_{BCS}\rangle$ gives us the $T << T_c$ K Cooper pair occupation function

$$v^2_{\mathbf{k}} = \frac{1}{2}[1 - \frac{E_0(\mathbf{k}) - E_F}{\sqrt{(E_0(\mathbf{k}) - E_F)^2 + \Delta^2}}], \quad (4)$$

where Δ is the *superconducting gap* given by $\Delta = -V_0 \sum_{\mathbf{k}} u_{\mathbf{k}} v_{\mathbf{k}}$. Make a plot of this function, and compare it with the single-particle non-interacting Fermi-Dirac function choosing appropriate numerical values.

(c) Using the earlier part on occupation functions, show that the *condensation energy*, or energy reduction for electrons to make a transition from the normal metallic to the superconducting state is $\mathcal{U}_{sc} - \mathcal{U}_m = -\frac{1}{2} N_0 \Delta^2$.

(d) I outlined in class how to obtain excited state properties from the BCS theory using the Bogoliubov de-Gennes approach instead of the variational approach. Show how this approach diagonalizes the BCS Hamiltonian in Equation 2 to the form

$$H_{BdG} = \sum_{\mathbf{k}} E_{BdG}(\mathbf{k})(\gamma^\dagger_{\mathbf{k}\uparrow}\gamma_{\mathbf{k}\uparrow} + \gamma^\dagger_{-\mathbf{k}\downarrow}\gamma^\dagger_{-\mathbf{k}\downarrow}), \quad (5)$$

where the quasiparticles have an energy spectrum $E_{BdG}(\mathbf{k}) = \sqrt{(E_0(\mathbf{k}) - E_F)^2 + \Delta^2}$. Write the relation between the creation/annihilation operators $\gamma_{\mathbf{k}}$'s and the original $c_{\mathbf{k}}$'s. Write the commutation relations of these new operators and comment.

(e) Outline how the temperature-dependent properties of the superconductor, say the gap $\Delta(T)$ may be obtained from the BCS type theory.

Solution: [By Sayak Ghosh (a), Ian Briggs (b, c, d) 2017]

4.4) a) Applying a voltage increases the number of right-going carriers over left-going carriers. Now, if there is enough voltage to excite electrons across superconducting gap Δ, Cooper pairs will start breaking up.

So, we need $\frac{\hbar^2}{2m^*}(k_R^2 - k_F^2) = \Delta$

$$\Rightarrow k_R^2 = \frac{2m^*\Delta}{\hbar^2} + k_F^2$$

$$\Rightarrow k_R \approx k_F\left(1 + \frac{\Delta m^*}{k_F^2 \hbar^2}\right).$$

Similarly, for electron number to stay same,

$$k_L \approx k_F\left(1 - \frac{\Delta m^*}{k_F^2 \hbar^2}\right)$$

Current density $J_c = n e \langle \vec{v} \rangle$

$$= n e \frac{\hbar (k_R - k_L)}{m^*}$$

$$= \frac{n e \hbar}{m^*} \cdot \frac{2\Delta m^* k_F}{k_F^2 \hbar^2}$$

$$= \frac{2 n e \Delta}{\hbar k_F}$$

using $n \sim 10^{27}\ m^{-3}$, $\Delta \sim 1\ meV$, $k_F \sim 10^{9}\ m^{-1}$ gives

$$J_c \approx 10^{11}\ A/m^2 = 10^{7}\ A/cm^2.$$

consider kinetic Energy picture

$\hat{H}_{eff} = \hat{H}_{tot} - E_F \qquad \varepsilon_k = E_0(k) - E_F$

$$\langle \Psi | \hat{H}_{eff} | \Psi \rangle = 2\sum_k \varepsilon_k v_k^2 - V_0 \sum_{k,k'} u_k v_k u_{k'} v_{k'}$$

$u_k^2 + v_k^2 = 1 \qquad u_k = \sin\theta_k \quad v_k = \cos\theta_k$

$$2\sum_k \varepsilon_k \cos^2\theta_k - V_0 \sum_k \sum_{k'} \sin\theta_k \cos\theta_k \sin\theta_{k'} \cos\theta_{k'}$$

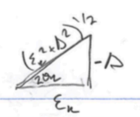
$$E(\theta_k) = \sum_k \varepsilon_k (1 + \cos(2\theta_k)) - \frac{V_0}{4} \sum_k \sum_{k'} \sin(2\theta_k)\sin(2\theta_{k'})$$

$$\frac{\partial E}{\partial \theta_k} = 0 = -2\varepsilon_k \sin(2\theta_k) - V_0 \sum_{k'} \cos(2\theta_k)\sin(2\theta_{k'})$$

$$\rightarrow \tan(2\theta_k) = -V_0 \sum_{k'} \frac{\sin(2\theta_{k'})}{2\varepsilon_k}$$

$$\Delta = -V_0 \sum_{k'} u_{k'} v_{k'} = -V_0 \sum_{k'} \sin\theta_{k'} \cos\theta_{k'} = -\frac{V_0}{2} \sum_{k'} \sin(2\theta_{k'})$$

$$\tan(2\theta_k) = \frac{2\Delta}{2\varepsilon_k} = \frac{\Delta}{\varepsilon_k}$$



$$\cos(2\theta_k) = -\frac{\varepsilon_k}{(\varepsilon_k^2 + \Delta^2)^{1/2}} = v_k^2 - u_k^2$$

$$v_k^2 + u_k^2 = 1$$

$$2v_k^2 = 1 - \frac{\varepsilon_k}{(\varepsilon_k^2 + \Delta^2)^{1/2}}$$

$$\rightarrow v_k^2 = \frac{1}{2}\left(1 - \frac{\varepsilon_k}{\sqrt{\varepsilon_k^2 + \Delta^2}}\right) \quad \varepsilon_k = E_0(k) - E_F \quad \checkmark\checkmark$$

$\Delta \sim 1\ meV$

c) $$\hat{H}_{eff} = \sum_{k\sigma} (E_0(k) - E_F)\hat{c}^\dagger_{k\sigma}\hat{c}_{k\sigma} - V_0 \sum_{k,q} \hat{c}^\dagger_{q\uparrow}\hat{c}^\dagger_{-q\downarrow}\hat{c}_{-k\downarrow}\hat{c}_{k\uparrow}$$

$$\langle \Psi | \hat{H}_{eff} | \Psi \rangle = \sum_k \left(\varepsilon_k - \frac{\varepsilon_k^2}{(\Delta^2 + \varepsilon_k^2)^{1/2}}\right) - \frac{\Delta^2}{V_0}$$

For normal metal: $\Delta = 0$

$$\langle \Psi | \hat{H}_{eff} | \Psi \rangle = \sum_{k,\sigma} \varepsilon_{k,\sigma} = \sum_k 2\varepsilon_k \quad (k \le k_F)$$

$= 0$ for $k > k_F$

$$\langle E \rangle_s - \langle E \rangle_n = \sum_{k > k_F}\left(\varepsilon_k - \frac{\varepsilon_k^2}{(\Delta^2 + \varepsilon_k^2)^{1/2}}\right) + \sum_{k \le k_F}\left(-\varepsilon_k - \frac{\varepsilon_k^2}{(\Delta^2 + \varepsilon_k^2)^{1/2}}\right)$$

$$= 2\sum_{k > k_F}\left(\varepsilon_k - \frac{\varepsilon_k^2}{(\varepsilon_k^2 + \Delta^2)^{1/2}}\right) - \frac{\Delta^2}{V_0} + \frac{\Delta^2}{V_0}$$

$$\approx \left[\frac{\Delta^2}{V} - \frac{1}{2}N_0\Delta^2\right] - \frac{\Delta^2}{V^2} = -\frac{1}{2}N_0\Delta^2 \quad \checkmark\checkmark$$

d) $$\hat{H}_{eff} = \sum_{k,\sigma} \varepsilon_k \hat{c}^\dagger_{k,\sigma}\hat{c}_{k,\sigma} - V_0 \sum_{k,q} \hat{c}^\dagger_{q\uparrow}\hat{c}^\dagger_{-q\downarrow}\hat{c}_{-k\downarrow}\hat{c}_{k\uparrow}$$

$$\hat{c}_{-k\downarrow}\hat{c}_{k\uparrow} = \hat{b}_k + (\hat{c}_{-k\downarrow}\hat{c}_{k\uparrow} - \hat{b}_k)$$

$$\hat{H}_m = \sum_{k\sigma} \varepsilon_k \hat{c}^\dagger_{k\sigma}\hat{c}_{k\sigma} - V_0 \sum_{k,k'} \hat{c}^\dagger_{k\uparrow}\hat{c}^\dagger_{-k\downarrow}\hat{b}_{k'} + \hat{b}^\dagger_k \hat{c}_{-k'\downarrow}\hat{c}_{k'\uparrow} - \hat{b}^\dagger_k \hat{b}_{k'}$$

where $b_k = \langle c_{-k\downarrow} c_{k\uparrow} \rangle$

$$\Delta = -\sum_k V_0 b_k = -V_0 \sum_k \langle c_{-k\downarrow} c_{k\uparrow} \rangle$$

$$H_m = \sum_{k,\sigma} \varepsilon_k \hat{c}^\dagger_{k\sigma}\hat{c}_{k\sigma} - \sum_k \Delta \hat{c}^\dagger_{k\uparrow}\hat{c}^\dagger_{-k\downarrow} + \Delta^* \hat{c}_{-k\downarrow}\hat{c}_{k\uparrow} - \Delta b_k^\dagger$$

$$\hat{c}_{k\uparrow} = u_k^* \gamma_{k\uparrow} + v_k \gamma^\dagger_{-k\downarrow} \qquad \hat{c}^\dagger_{-k\downarrow} = -v_k^* \gamma_{k\uparrow} + u_k \gamma^\dagger_{-k\downarrow}$$

$$|u_k|^2 + |v_k|^2 = 1$$

$$H_m = \sum_k \varepsilon_k \Big[(|u_k|^2 - |v_k|^2)(\gamma^\dagger_{k\uparrow}\gamma_{k\uparrow} + \gamma^\dagger_{-k\downarrow}\gamma_{-k\downarrow}) + 2|v_k|^2 + 2u_k^* v_k^* \gamma_{-k\downarrow}\gamma_{k\uparrow}$$

$$+ 2u_k v_k \gamma^\dagger_{k\uparrow}\gamma^\dagger_{-k\downarrow}\Big] + \sum_k \Big[(\Delta u_k v_k^* + \Delta^* u_k^* v_k)(\gamma^\dagger_{k\uparrow}\gamma_{k\uparrow} + \gamma^\dagger_{-k\downarrow}\gamma_{-k\downarrow} - 1)$$

$$+ (\Delta v_k^{*2} - \Delta u_k^{*2})\gamma_{-k\downarrow}\gamma_{k\uparrow} + (\Delta^* v_k^2 - \Delta u_k^2)\gamma^\dagger_{k\uparrow}\gamma^\dagger_{-k\downarrow} + \Delta b_k^\dagger\Big]$$

diagonalizes (only $\gamma_k^\dagger \gamma_k$ terms) when

$$2\varepsilon_k u_k v_k + \Delta^* v_k^2 - \Delta u_k^2 = 0$$

$$\Rightarrow v_k^2 = \frac{1}{2}\left(1 - \frac{\varepsilon_k}{(\Delta^2 + \varepsilon_k^2)^{1/2}}\right) \quad \checkmark\checkmark$$

$\rightarrow H_m = \sum_k E_k(\gamma^+_{k\uparrow}\gamma_{k\uparrow} + \gamma^+_{-k\downarrow}\gamma_{-k\downarrow})$

where $E_k = (\xi_k^2 + \Delta^2)^{1/2}$

$\{\hat{c}, \hat{c}^+\} = 1$

$\{\hat{c}_{k\uparrow}, \hat{c}^+_{k\uparrow}\} = 1$

$\{u_k^*\gamma_{k\uparrow} + v_k\gamma^+_{-k\downarrow},\ u_k\gamma^+_{k\uparrow} + v_k^*\gamma_{-k\downarrow}\} = 1$

$\{A+B, C+D\} = (A+B)(C+D) + (C+D)(A+B)$
$= (AC+CA) + (BC+CB) + (AD+DA) + (BD+DB)$
$= \{A,C\} + \{B,C\} + \{A,D\} + \{B,D\}$

$\{u_k^*\gamma_{k\uparrow}, u_k\gamma^+_{k\uparrow}\} + \{v_k\gamma^+_{-k\downarrow}, u_k\gamma^+_{k\uparrow}\} + \{u_k^*\gamma_{k\uparrow}, v_k^*\gamma_{-k\downarrow}\}$
$+ \{v_k\gamma^+_{-k\downarrow}, v_k^*\gamma_{-k\downarrow}\} = 1$

$\hat{c}_{k\uparrow} = u_k^*\gamma_{k\uparrow} + v_k\gamma^+_{-k\downarrow}$ $\qquad$ ~~$\hat{c}_{k\uparrow} = u_k^*\gamma_{k\uparrow} + v_k\gamma_{k\downarrow}$~~

$\frac{u_k^*}{v_k^*}(\hat{c}^+_{-k\downarrow} = -v_k^*\gamma_{k\uparrow} + u_k\gamma^+_{-k\downarrow})$ $\qquad$ ~~$\frac{u_k^*}{v_k^*}\hat{c}^+_{-k\downarrow} = -u_k^*\gamma_{k\uparrow} + \frac{u_k^* u_k}{v_k^*}\gamma^+_{-k\downarrow}$~~

$\hat{c}_{k\uparrow} + \frac{u_k^*}{v_k^*}\hat{c}^+_{-k\downarrow} = \left(v_k + \frac{|u_k|^2}{v_k^*}\right)\gamma^+_{-k\downarrow} = \left(\frac{v_k v_k^*}{v_k^*} + \frac{|u_k|^2}{v_k^*}\right)\gamma^+_{-k\downarrow}$

$\hat{c}_{k\uparrow} + \frac{u_k^*}{v_k^*}\hat{c}^+_{-k\downarrow} = \frac{|v_k|^2 + |u_k|^2}{v_k^*}\gamma^+_{-k\downarrow} = \frac{1}{v_k^*}\gamma^+_{-k\downarrow}$

$\gamma^+_{-k\downarrow} = v_k^*\hat{c}_{k\uparrow} + u_k^*\hat{c}^+_{-k\downarrow}$ $\qquad$ $\gamma_{-k\downarrow} = v_k\hat{c}^+_{k\uparrow} + u_k\hat{c}_{-k\downarrow}$

$\{\gamma_{-k\downarrow}, \gamma^+_{-k\downarrow}\} = \{v_k\hat{c}^+_{k\uparrow} + u_k\hat{c}_{-k\downarrow},\ v_k^*\hat{c}_{k\uparrow} + u_k^*\hat{c}^+_{-k\downarrow}\}$
$= \{v_k\hat{c}^+_{k\uparrow}, v_k^*\hat{c}_{k\uparrow}\} + \{u_k\hat{c}_{-k\downarrow}, u_k^*\hat{c}^+_{-k\downarrow}\}$
$= |v_k|^2\{c^+_{k\uparrow}, c_{k\uparrow}\} + |u_k|^2\{\hat{c}_{-k\downarrow}, \hat{c}^+_{-k\downarrow}\} = 1$

$\{\gamma_{-k\downarrow}, \gamma^+_{-k\downarrow}\} = 1 \qquad \{\gamma^+_{-k\downarrow}, \gamma^+_{-k\downarrow}\} = 0$

$\{\gamma_{-k\downarrow}, \gamma_{-k\downarrow}\} = 0$

$\hat{c}_{k\uparrow} = u_k^*\gamma_{k\uparrow} + v_k(v_k^*\hat{c}_{k\uparrow} + u_k^*\hat{c}^+_{-k\downarrow})$

$\hat{c}_{k\uparrow} = u_k^*\gamma_{k\uparrow} + |v_k|^2\hat{c}_{k\uparrow} + v_k u_k^*\hat{c}^+_{-k\downarrow}$

$u_k^*\gamma_{k\uparrow} = \underbrace{(1-|v_k|^2)}_{|u_k|^2}\hat{c}_{k\uparrow} - v_k u_k^*\hat{c}^+_{-k\downarrow}$

$\gamma_{k\uparrow} = u_k\hat{c}_{k\uparrow} - v_k\hat{c}^+_{-k\downarrow}$

$\gamma^+_{k\uparrow} = u_k^*\hat{c}^+_{k\uparrow} - v_k^*\hat{c}_{-k\downarrow}$

$\{\gamma_{k\uparrow}, \gamma^+_{k\uparrow}\} = \{u_k\hat{c}_{k\uparrow} - v_k\hat{c}^+_{-k\downarrow},\ u_k^*\hat{c}^+_{k\uparrow} - v_k^*\hat{c}_{-k\downarrow}\}$
$= 1$

$\{\gamma_{k\uparrow}, \gamma_{k\uparrow}\} = 0 \qquad \{\gamma^+_{k\uparrow}, \gamma^+_{k\uparrow}\} = 0$

γ_k operators have commutative properties of fermions

e) quasi-fermionic particles from excitation follow fermi distribution of occupation probability

$f(E_k) = \frac{1}{1+e^{\beta E_k}} \qquad \beta = 1/kT$

$(E_k = (\xi_k^2 + \Delta^2)^{1/2})$

$\langle 1 - \gamma^+_{k\uparrow}\gamma_{k\uparrow} - \gamma^+_{-k\downarrow}\gamma_{-k\downarrow}\rangle = 1 - 2f(E_k)$

$\Delta = -V_0\sum_k u_k^* v_k[1 - 2f(E_k)]$

$\Delta = -\sum_k \frac{V_0\Delta}{2E_k}\tanh\left(\frac{\beta E_k}{2}\right)$

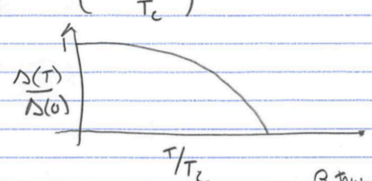
$\rightarrow \frac{1}{V} = \frac{1}{2}\sum_k \frac{\tanh(\beta E_k/2)}{E_k} = \frac{1}{2}\sum_k \frac{\tanh(\beta(\xi_k^2+\Delta^2)^{1/2}/2)}{(\xi_k^2+\Delta^2)^{1/2}}$

use this eqn to solve for E_k as a function of β

$\rightarrow$ converting summation into integral

$$\frac{1}{N(0)V} = \int_0^{\hbar\omega_c} \frac{\tanh\left(\frac{1}{2}\beta(\varepsilon_k^2 + \Delta^2)^{1/2}\right) d\varepsilon}{(\varepsilon^2 + \Delta^2)^{1/2}}$$

$\frac{\Delta(T)}{\Delta(0)} \approx 1.74\left(1 - \frac{T}{T_c}\right)^{1/2}$ for T near T_c



determining T_c: $(\Delta = 0)$ $\quad \frac{1}{N(0)V} = \int_0^{\beta_c\hbar\omega_c/2} \frac{\tanh(x)}{x}dx$

$\rightarrow kT_c = 1.13\hbar\omega_c e^{-1/N(0)V}$