Department Of Physics

DUAL DEGREE PROJECT

Characterization of Superconductor Junctions

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Abstract

Topological quantum matter has emerged as an exciting field in the last decade. From hosting topologically protected surface states, to possessing potential to for fault tolerant quantum computing, topology has infused a rich physics into conventional band theory. Transport wise, interesting properties reveal when a topological insulator is kept in proximity to superconductor forming a hyrbid structure. In such hybrids, the presence of a magnetic field or a magnetic moment of an adjacent ferromagnet can spawn zero energy Majorana modes, the focus of much of current research in quantum computing.

With this background, this thesis aims to study characteristics of Superconductor - Topological junctions, particularly the effect of surface states on superconducting parameters such as transition temperatures, critical fields. For the time being, we focus on T_c to see how the non-zero density of surface states influences its value, the interplay of coherence length with decay length, and how material aspect ratios influences T_c. By reformulating an older method by de Gennes [1], our approach can possibly yield a simpler methodology to compute T_c as compared to other methods such as quasiclassical green's function.

Contents

Chapter 1

Setup: Superconductivity in inhomogenous systems

In this chapter, we review some of the basics of conventional BCS, modified to account for inhomogenity. This would serve as preparation for next chapter, where we linearize these equations.

1.0.1 BCS theory

To derive order parameter $\Delta(\vec{r})$ and excitation spectrum, one uses mean field method of treating the pairing term in conventional BCS theory. One particular assumption is that of "contact potential" - assume that the electrons are interacting by a potential of the form $V(\vec{r}_1.\vec{r}_2) = -V(\vec{r}_1)\delta^3(\vec{r}_2 - \vec{r}_2)$. However, the more correct statement is as follows:

We take the BCS hamiltonian to be

$$H_{BCS} = \sum_{\vec{k},\sigma} \epsilon(\vec{k})\ c^\dagger_{\vec{k},\sigma} c_{\vec{k},\sigma} - \frac{g}{V} \sum_{\vec{k},\vec{q}} c^\dagger_{\vec{k},\uparrow} c^\dagger_{-\vec{k},\downarrow} c_{-\vec{q},\downarrow} c_{\vec{q},\uparrow}$$

Where g is a positive constant. The Hamiltonian H_{BCS} should be interpreted as an effective Hamiltonian describing the physics of a thin shell of states of width $O(_d)$ centered around the Fermi surface (i.e. the region where a net attractive interaction prevails). One should keep in mind that there is an implicit assumption of $|\xi_k|, |\xi_q| < \omega_d$ in the 2nd term, something that's generally inserted once energy integrals are done.

1.0.2 Derivation of BdG equations in inhomogeneous systems

Since inhomogeneous systems don't have translational symmetry, standard BCS theory written in momentum space (see Tinkham) need to be modified.

We try with a real space formulation of standard BCS theory

$$H_{BCS} = \int \psi^\dagger(\vec{r},\sigma) H_0(\vec{\mathbf{r}}) \psi(\vec{\mathbf{r}},\sigma) - V \int \psi^\dagger(\vec{r},\uparrow)\psi^\dagger(\vec{r},\downarrow)\psi(\vec{r},\downarrow)\psi(\vec{r},\uparrow)$$

where V is the (positive) strength of the BCS interaction. Now doing MFT with it gives

$$H_{MF} = \int \psi^\dagger(\vec{r},\sigma) H_0(\vec{\mathbf{r}}) \psi(\vec{\mathbf{r}},\sigma) + \int \left(\Delta(\vec{\mathbf{r}})\ \psi^\dagger(\vec{r},\uparrow)\psi^\dagger(\vec{r},\downarrow) + \Delta^*(\vec{\mathbf{r}})\ \psi(\vec{r},\downarrow)\psi(\vec{r},\uparrow) \right)$$

where $H_0(\vec{\mathbf{r}}) = \hat{p}^2/2m + U(\vec{\mathbf{r}}) - \mu$, $\Delta(\vec{\mathbf{r}}) = -V\langle\psi(\vec{r},\downarrow)\psi(\vec{r},\uparrow)\rangle$ ($U(\vec{\mathbf{r}})$ being one-electron potential, added to account for impurities).

Now we try the usual prescription to diagonalize the quadratic hamiltonian by introducing new fermionic operators

$$\psi(\vec{r},\uparrow) = \sum_n (u_n\gamma_{n,\uparrow} - v_n^*\gamma_{n,\downarrow}^\dagger) \tag{1.1}$$

$$\psi(\vec{r},\downarrow) = \sum_n (\gamma_{n,\downarrow}u_n + \gamma_{n,\uparrow}^\dagger v_n^*) \tag{1.2}$$

with the usual fermionic commutation relation given by $\{\gamma_{n,\sigma}, \gamma_{m,\sigma'}\} = \delta_{nm,\sigma\sigma'}$. (here n,m are quantum numbers for different eigenstates of Quasiparticles). The resulting hamitltonian looks as

$$H_{MF} = E_g + \sum_n \epsilon_n \gamma_{n,\sigma}^\dagger \gamma_{n,\sigma}$$

Brief aside: There are multiple ways to do bogoliubov trasnformation. Each way is unique to the problem at hand and more often than not, there are additional pieces alongside BCS hamiltonian. Transformation must diagonalize these pieces too. For a simple example, Tinkham does the following transformation

$$c_{k\uparrow} = u_k^*\gamma_{k0} + v_k\gamma_{k1}^\dagger \tag{1.3}$$

$$c_{-k\downarrow} = u_k^*\gamma_{k1} - v_k\gamma_{k0}^\dagger \tag{1.4}$$

What are 1 & 2? They're analogous to spin up and down (which is what we've used in the our previous bog. transf.) The point to note is that all such bogoliubov trasnformation generally encompass two things -

- They trade up and down spin for two 1,2 or up, down quasiparticles
- Transformations generally differ by a -ve sign, when comparing $k\uparrow \;\; -k\downarrow$

How do we determine what $u_n(r), v_n(r)$ actually are? The idea is to use $[H_{MF}, \psi], [H_{MF}, \gamma]$ and then equate each other through relations (1.1), (1.2). This leads to **BdG Equations** given by

$$\begin{pmatrix} H_0(\vec{\mathbf{r}}) & \Delta(\vec{\mathbf{r}}) \\ \Delta^*(\vec{\mathbf{r}}) & -H_0^*(\vec{\mathbf{r}}) \end{pmatrix} \begin{pmatrix} u_n(\vec{\mathbf{r}}) \\ v_n(\vec{\mathbf{r}}) \end{pmatrix} = \epsilon_n \begin{pmatrix} u_n(\vec{\mathbf{r}}) \\ v_n(\vec{\mathbf{r}}) \end{pmatrix} \tag{1.5}$$

- Caution: u,v appearing here are not to be confused with u_k, v_k that appears in BCS GS wavefunction. The latter doesn't bear a simple relation to the former at all. For more on this and an interesting relation between both, see AJ legget's course notes.
- The matrix in eqn (1.5)is quite insightful: looking at the diagonal entries, we see that a hole hamiltonian is obtained from an electron hamiltionian by :
  - First by changing the sign of H i.e. energy of a hole is equal to negative of energy of a particle.

  - Then doing $H \to H^*$ i.e. a version of quantum time reversal operation (this sets $\hat{p} \to -\hat{p}$ $\hat{x} \to \hat{x}$). This is completely in lieu with the idea that a hole or antiparticle can be imagined as a particle travelling backward in time. It is therefore quite natural to interpret u_n as the particle and v_n as the hole parts of the 2 component spinor.

- BdG equation is an eigenvalue equation of the form $\hat{\Omega}\begin{pmatrix} u_n \\ v_n \end{pmatrix} = \epsilon_n \begin{pmatrix} u_n \\ v_n \end{pmatrix}$, where $\hat{\Omega}$ being hermitian guarantees the orthogonality of $\begin{pmatrix} u_n \\ v_n \end{pmatrix}$.

- It can be shown that for every solution $\begin{pmatrix} u_n \\ v_n \end{pmatrix}$ with eigenvalue ϵ_n, we have another solution $\begin{pmatrix} -v_n^* \\ u_n^* \end{pmatrix}$ with eigenvalue $-\epsilon_n$.

- This is a so-called particle-hole symmetry, which is an instrinsic property of BCS mean field hamiltonian (but in no way of the original H). It lies in the fact that relation (1.0.2) doesn't uniquely define the operator γ or the constant E_g. This is verified by defining new operators $\hat{\Gamma} = \gamma^\dagger$ and rewriting (1.0.2) in terms of $\hat{\Gamma}$, to obtain the same relation but with different constant E' and operators. (infact from previous point, we see that the difference term of $\sum_n \epsilon_n = 0$, so $E' = E_g$)

- Accordingly, the local pairing potential $\Delta(\vec{\mathbf{r}})$ can be determined by using $\Delta(\vec{\mathbf{r}}) = -V\langle\psi(\vec{r},\downarrow)\psi(\vec{r},\uparrow)\rangle$, putting $\psi \to \gamma$ and using the mean value of $< \gamma^\dagger\gamma >= n_{fermi}(\epsilon_n)$ (no chemical potential occurs here for the bogoliubov particles as they can created as well as destroyed i.e. they don't have fixed number. cf. Phonons). This yields (and this solution is explicit for the case of contact potential $-V\delta(r)$) as

$$\boxed{\Delta(\vec{r}) = V\sum_n v_n^*(\vec{\mathbf{r}})u_n(\vec{\mathbf{r}})\ tanh(\beta E_n/2)}$$

  This leads to a non-linear self-consistent set of equations taken with (1.0.2). To ensure convergence, one generally cuts V when ϵ_n (excitation energy when $\Delta = 0$ i.e. no coupling of particle hole branch) is higher than ω_d.

- Normalization: Eigenvalues ϵ_n are independent of normalisation, however, $\Delta(\vec{\mathbf{r}})$ is dependent on it. We implicitly have chosen the normalization $\int |u_n(\vec{\mathbf{r}})|^2 + |v_n(\vec{\mathbf{r}})|^2\ d\vec{\mathbf{r}} = 1$

For a more general derivation of BdG equation with a general potential $V(\vec{\mathbf{r}}_1 - \vec{\mathbf{r}}_2)$ instead of the contact potential, checkout the 1st chapter of the book "Bogoliubov-deGennes Method and Its Applications" by Jian-Xin Zhu.

For completeness, we workout the solution to BdG in some special cases .

1.0.3 Examples

Case 1: Uniform Homogenous superconductor in absence of a magnetic field

Because of translational invariance, the quasi-particle eigenstates i.e. n = $\vec{\mathbf{k}}\tilde{\alpha}$, where $\vec{\mathbf{k}}$ is the wave-vector while the spin index- $\tilde{\alpha}$ is generally some linear combination of usual spin-index $\alpha = \uparrow, \downarrow$. Now, from definition $\Delta(\vec{\mathbf{r}}) = -V\langle\psi(\vec{r},\downarrow)\psi(\vec{r},\uparrow)\rangle$, we can see that any average $\langle\psi(\vec{\mathbf{r}}_1)\psi(\vec{\mathbf{r}}_2)\rangle \sim f(\vec{r_1} - \vec{r_2})$ in lieu of translational invariance, therefore $\Delta(\vec{\mathbf{r}}) = \Delta = const.$ Moreover, the normalisation condition now reduces to $|u_k|^2 + |v_k|^2 = 1$.

We set $\begin{pmatrix} u_n(\vec{\mathbf{r}}) \\ v_n(\vec{\mathbf{r}}) \end{pmatrix} = \begin{pmatrix} u_k(\vec{\mathbf{r}}) \\ v_k(\vec{\mathbf{r}}) \end{pmatrix} = \frac{e^{ikr}}{\sqrt{V_{solid}}} \begin{pmatrix} u_k \\ v_k \end{pmatrix}$ as our solution. Solving for eigenenergies E is now straight-forward as we have

$\hat{H}_{BdG} = \hat{\Omega}(\vec{\mathbf{k}}) = \begin{pmatrix} \xi_k & \Delta \\ \Delta^* & -\xi_k \end{pmatrix} \implies E_{\pm}(\vec{\mathbf{k}}) = \pm\sqrt{\xi_k^2 + |\Delta|^2}$ (we only take the positive energy branch as excitation energies) .

To find eigenvectors, we redefine the matrix $\hat{\Omega}/|E| = \begin{pmatrix} cos(\theta_k) & sin(\theta_k)e^{i\phi_k} \\ sin(\theta_k)e^{-i\phi_k} & -cos(\theta_k) \end{pmatrix}$, where ϕ_k is the phase of Δ.

We can read off the eigenvectors as $\psi_+ = \begin{pmatrix} cos(\theta_k/2)e^{i\phi_k} \\ sin(\theta_k/2) \end{pmatrix}$ $\psi_- = \begin{pmatrix} sin(\theta_k/2) \\ -cos(\theta_k/2)e^{-i\phi_k} \end{pmatrix}$. This parametrisation has the advantage that given ψ_+ , one extracts ψ_- by applying the TR operator and that the normalisation condition is manifestedly satisfied. Explicitly we have

$$\begin{pmatrix} \sqrt{\frac{1}{2}\left(1 + \frac{\xi_k}{E_k}\right)}e^{i\phi_k} \\ \sqrt{\frac{1}{2}\left(1 - \frac{\xi_k}{E_k}\right)} \end{pmatrix} \psi_- = \begin{pmatrix} \sqrt{\frac{1}{2}\left(1 - \frac{\xi_k}{E_k}\right)} \\ -\sqrt{\frac{1}{2}\left(1 + \frac{\xi_k}{E_k}\right)}e^{-i\phi_k} \end{pmatrix} \tag{1.6}$$

Physically, quasi-particle states are plane waves, with u_k, v_k being the electron and hole components of it. But what about the gap Δ?

This has to be calculated self-consistently as

$$\Delta = V\sum_k v_k^* u_k \; tanh(\frac{\beta E_k}{2})$$

At this point, we put a cutoff on the k-summation here (which is in no way explcit) b/w [-ω_d,ω_d] of E_F. The more general eqauation is given by

$$\Delta(r, r') = V(r - r')\sum_n u_n(r)v_n^*(r') \; tanh(\frac{\beta E_n}{2}) \tag{1.7}$$

where now the definition of the pairing potential is given by $\Delta(r, r') = -v(r - r')\langle\psi_\downarrow(r)\psi_\uparrow(r')\rangle$ whence the contribution to H_{MF} comes as $\int_r\int_{r'}\Delta(r, r')\psi_\uparrow^\dagger(r)\psi_\downarrow^\dagger(r') + h.c.$ Now putting a contact interaction (so that $r' = r$ in (1.7)) and imposing translational invariance (so that $\Delta(r, r') = \Delta(r - r')$ $u_k(r) \sim e^{ikr}u_k$, $v_k^*(r) \sim e^{-kr}v_k$ cancelling out the r dependence in (1.7)) will give us back ((1.6)).

But to see the idea of putting cutoff explicitly, let's not put a contact interaction and instead put the shell-like interaction as done by Cooper with cutoff ω_D . Now in k-space ((1.7)) looks like

$$\frac{1}{V_{solid}}\int_r\int_{r'}\Delta(r,r')e^{-ik(r-r')} = V_{\vec{\mathbf{k}},\vec{\mathbf{q}}}u_n(\vec{\mathbf{q}})v_n^*(\vec{\mathbf{q}})\ tanh(\frac{\beta E_q}{2})$$

where $V_{k,q}$ is the matrix element $\langle k,-k|V|q,-q\rangle$. We've simply done a f.t. until now but upon demanding translational invariance, we we get

$$\Delta_k = V_{k,q}\ u_q v_q^*\ tanh(\frac{\beta E_q}{2})$$

with $\Delta_k = \int_r \Delta(r)e^{-ikr}$. Now à la Cooper we set $V_{k,q} = V_0$ but only for $|\xi_k|, |\xi_q| \leq \omega_d$. Now we get (note that this sets $\Delta_k = \Delta$)

$$\Delta = Vu_q v_q^*\ tanh(\frac{\beta E_q}{2}) \tag{1.8}$$

$$\implies \Delta = V\int\frac{d\vec{\mathbf{k}}}{(2\pi)^3}\frac{\Delta}{2E_k}tanh(\frac{\beta E_k}{2}) \tag{1.9}$$

$$\implies 1 = V\int g(\epsilon)d\epsilon\frac{1}{2\sqrt{\Delta^2+(\epsilon-\mu)^2}}tanh\left(\frac{\beta\sqrt{\Delta^2+(\epsilon-\mu)^2}}{2}\right) \tag{1.10}$$

$$\implies 1 = \frac{g(\epsilon_F)V}{2}\int_{-\omega_d}^{\omega_d}d\xi\frac{1}{\sqrt{\Delta^2+\xi^2}}tanh\left(\frac{\beta\sqrt{\Delta^2+\xi^2}}{2}\right) \tag{1.11}$$

$$\xrightarrow{T=0\ limit}\quad 1 = \frac{g(\epsilon_F)V}{1}\int_0^{\omega_d}d\xi\frac{1}{\sqrt{\Delta^2+\xi^2}}\frac{\pi}{2} \tag{1.12}$$

which gives back $\Delta \sim 2\omega_d exp(-\frac{1}{g(\epsilon_F)*V})$

Now similarly as (1.12) we can workout (1.0.3) too to arrive at similar result (i.e. gap to 0K and T_c). This then completes the calculation of the pair potential. One can also calculate dos using this (done in Zhu's book eqn 1.125).

Case 2: Uniform homogenous Superconductor with a uniform current flow

We want to analyze the quasi-particle spectrum for a state of uniform current dlow, in a pure superconductor. A state of uniform flow is described by a pair potential ofthe form $\Delta = |\Delta|e^{2i\vec{\mathbf{q}}\cdot\vec{\mathbf{r}}}$, where $\vec{\mathbf{q}}$ is a vector on the direction of flow (the average momentum per electron in this state is $\hbar\vec{\mathbf{q}}$).

To proceed, we just modify our homogenous solution by setting $u_k(r) = e^{i(k+q)r}u_k$ and $v_k(r) = v_k e^{i(k-q)r}$. Then H_{BdG} becomes

$$\begin{pmatrix}\frac{(k+q)^2}{2m}-\mu & |\Delta| \\ |\Delta| & \frac{(k-q)^2}{2m}-\mu\end{pmatrix} = |\Delta|\sigma_x + (\epsilon_q+\xi_k)\sigma_z + \frac{\vec{\mathbf{k}}\cdot\vec{\mathbf{q}}}{m} \tag{1.13}$$

$$\implies E_\pm(\vec{\mathbf{k}}) = \pm\sqrt{|\Delta|^2+(\xi_k+\epsilon_q)^2}+\frac{\vec{\mathbf{k}}\cdot\vec{\mathbf{q}}}{m} \tag{1.14}$$

$$\xrightarrow[taking\ positive\ eigenvalue]{retaining\ terms\ upto\ first\ order\ in\ q} E^0(k)+\frac{\vec{\mathbf{k}}\cdot\vec{\mathbf{q}}}{m} \tag{1.15}$$

We're interesed in the following case (which also explains the retainment of linear order only): Suppose $q \sim \frac{\Delta}{\hbar k_F}$, then $q \ll k_F$. Now we can see that it's possible that the quasi-particle gap can turn 0. However, keep in mind that $\Delta = f(v_s)$ too, through self-consistent calculation.

Chapter 2

Superconductor - Normal Junctions: Perturbative expansion near T_C

2.1 Introduction

In this chapter, we study T_c of superconductor-normal metal junctions. Specifically, this is a note on the paper titled "*Boundary Effects in Superconductors*" by P.G.de Gennes (1964)[1]. The main summary of the paper is as follows:

- It deals with finite size effects of NS junctions in observable T_c
- The paper specifically focuses on dirty S - dirty N junction (leaving the clean case aside)
- Using a linearized BdG equation with small Δ near T_c, it tries to get analytic solutions to T_c for different situations.

2.2 Order Parameter and Excitation Spectrum in a non-homogenous system

For the S-N junction, the value of the pairing strength g (or V_s in the paper) is necessarily positive while in metal $g_N = V_N$ can either be positive or negative(repulsive interaction) depending on competition between Coulomb repulsion and phonon-induced interaction.

When $V_N > 0$, we get a S-S junction at temperatures $T < T_{c,normal}$ corresp to normal side superconducting. However, if the strength is small i.e. $V_N \lessapprox \frac{V_s}{2}$, then transition temperature becomes so small for the normal side that we never observe it. It is in this sense that this paper allows for S-N description, even though nåively one might think it's really an S-S junction.

Using this hamiltonian, we can derive the excitation spectrum. Restating the BdG equations from previous chapter

$$\begin{pmatrix} H_0(\vec{\mathbf{r}}) & \Delta(\vec{\mathbf{r}}) \\ \Delta^*(\vec{\mathbf{r}}) & -H_0^*(\vec{\mathbf{r}}) \end{pmatrix} \begin{pmatrix} u_n(\vec{\mathbf{r}}) \\ v_n(\vec{\mathbf{r}}) \end{pmatrix} = \epsilon_n \begin{pmatrix} u_n(\vec{\mathbf{r}}) \\ v_n(\vec{\mathbf{r}}) \end{pmatrix} \tag{2.1}$$

The spatial dependence of Δ has some important consequences:

1. We can no longer have u_n, v_n be proportional to one-electron wavefunctions in the normal metal that solve the eigenvalue problem $(p^2/2m+U(r))\ w_n(r) = \epsilon_n w_n(r)$. This would be so if Δ were space independent (solution for homogenous SC). Physically, this culminates from the fact that it's not optimal for the system to pair an electron in state w_n and time-reversed state $\mathcal{T}w_n$ together while making a bound pair.

2. We expect a variation of this kind:

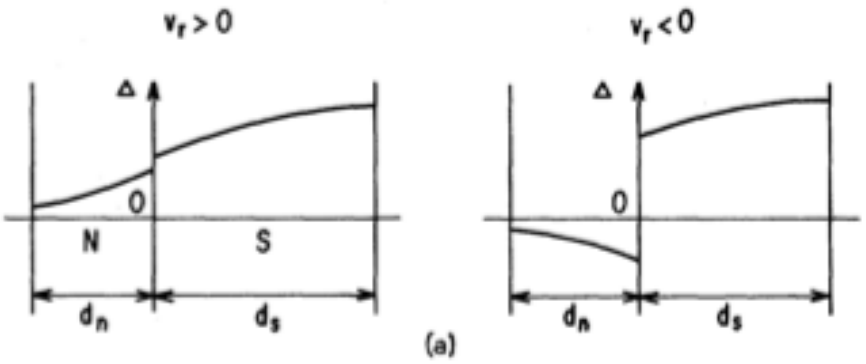

Figure 2.1: Variation of pair potential $\Delta(x)$.Two cases of V_N >0 and < 0 have been shown. Taken from [1]
Diagram on LHS is for when $V_N > 0$ (i.e. metal is a SC) and RHS is for $V_N < 0$ i.e. metal has repulsive interactions.

3. Boundary Conditions: On microscopic scale, we've $\Delta(r)$, $F(r) = \langle \psi_\uparrow(r)\psi_\downarrow(r) \rangle$ are continuous. But when we model the interface between two metals as a sharp boundary, neither F, nor Δ is continouous across this surface. It'll be proven that the quantity that remains continuous is $F(r)/N(r) = \Delta(r)/(N(r) * V(r))$ where $N(r)$ is the local density of states (per unit real volume, per unit energy) at the fermi level.

4. Theorem : If $\Delta(r)$ depends only on 1-coordinate, then the energy gap E_0 (which is the minimum energy required to excite a quasi-particle) is equal to **minimum** value of $\Delta(r)$ in the sample.

2.3 Self-Consistent Solution to the pair potential

The naive method to solve BdG equations is to guess a shape of $\Delta(x)$, use that to calculate u,v and then use the resulting u's and v's in the self-consistency requirement, obtain a new value for Δ(x) and iterate the process. However, this strategy is

cumbersome and difficult to implement. It turns out to determine T_c, there is a great simplification that can be done which goes as follows:

In order to determine T_c, work near T_c. Assuming the system still exhibits a second order phase transition, now we have a small Δ, which enables us to treat it as a perturbation in the BdG eigenvalue equation. Using that, we calculate u,v perturbatively and then plug it back into self consistency equation. Now self-consistent equation looks of the form $\Delta = f(u, v, T)$, where u, v themselves depend on Δ (BdG eqn). It becomes now possible to linearize the self-consistency equation. Because this dependence is now linear, this engenders a fighting chance of solving the equation analytically and determining Δ, T_c . This is the principal strategy employed in [1].

This derivation is carried out in **Appendix**, mostly drawing from [1] and Ch7 of de Gennes book on Superconductivity. The main results are re-stated as

- $\Delta(r)$ obeys
$$\Delta(r) = V(r) \sum_{\omega} \int d^3r' H_\omega(\vec{\mathbf{r}}, \vec{\mathbf{r}}')\Delta(\vec{\mathbf{r}}')$$
where $H_\omega(r, r')$ acts as a kernel.

- $H_\omega(r, r')$ is defined by
$$H_\omega(r, r') = T \sum_{n,m} \frac{1}{\epsilon_n - i\omega} \times \frac{1}{\epsilon_m + i\omega} \times w_m^*(r) w_n^*(r) w_n(r') w_m(r')$$
where $\omega = (2k + 1)\pi/\beta$ i.e. fermionic matsubara frequencies, ϵ_m being the eigenvalues for non-interacting hamiltonian $\hat{\mathcal{H}} = p^2/2m + U$, while $w_m(r)$ are the corresponding wavefunctions. These include effects of impurities/boundaries through $U(r)$. Further, we choose w_n to be real (which amounts to choosing standing wave instead of a travelling wave solution. This is possible since $\hat{\mathcal{H}}$ is real).

One additional property that the kernel $H_\omega(r, r')$ follows is the **sum rule**. This refers to the fact that

$$\int H_\omega(r, r')dr' = \sum_n \frac{1}{\epsilon_n^2 + \omega^2} |w_n(r)|^2 \tag{2.2}$$

$$= N(r) \int \frac{d\epsilon}{\epsilon^2 + \omega^2} = N(r) \frac{\pi}{|\omega|} \tag{2.3}$$

The last result needs some interpretation. Here, rather implicitly, sum over ϵ_n is carried at the fermi level, and hence naturally we have $N(r)$ as the local density of state at the fermi level (because of the dangling $|w_n(\vec{\mathbf{r}})|^2$) present. Doing the energy integral for states at the fermi level i.e. b/w $-\omega_d, \omega_d$ and assuming that $\omega_D \gg T_c$, we get the final final result (where ω_d doesn't appear).

One can re-write the kernel in terms of a one-correlation function defined by the relation

$$G_\Omega(rr') = \sum_m \overline{w_n(r)w_m(r)w_n(r')w_m(r')}\delta(\epsilon_n - \epsilon_m + \Omega) \tag{2.4}$$

$$\implies G(rr't) = \int \frac{dt}{2\pi} e^{i\Omega t} G_\Omega(rr') \tag{2.5}$$

$$\implies G(rr't) = \overline{\delta(\hat{r}(0) - r)\delta(\hat{r}(t) - r')} \tag{2.6}$$

where the last line can be checked simply by using the integral representation of the δ function. Also, as is derived in appendix, the average is done over all states w_n with fixed energy (fermi energy for the current paper). Once $G(r, r', t)$ is known, then one can just the full kernel K_0 in terms of it using (2.3).

When the electron mean free path is small, then the correlation function (2.6) spreads according to a diffusion equation

$$\frac{\partial G(rr't)}{\partial |t|} - D\nabla^2 G(rr't) = const \times \delta(rr')\delta(t)$$

Here $D = 1/3v_F l$. This form makes $G(rr't)$ the Green's function for the diffusion equation. This holds when $|r - r'| \gg \lambda_F$ (i.e. uncertainty relations don't come into play) and diffusion approximation works ($|r - r'| \gg l$ and $t \gg l/v_F$). Now as done in following derivation, one can extract fourier components of G from the above equation and then correspondingly derive the fourier components of $H_\omega(r, r')$ as well. Stating the final result, we've

$$H_\omega(x, x') = \frac{\pi N}{2|\omega|\xi_\omega} e^{-|x-x'|/\xi_\omega}$$

where $\xi_\omega = (D/2|\omega|)^{1/2}$. And consequently, the largest range corresponds to $|\omega| = \pi k_B T$, which gives the said coherence length of the material (as in (A.0.5)) as $\xi = \sqrt{(\frac{D}{2\pi T})}$.

Chapter 3

Application: Superconductor - Topological Insulator Junctions

In this chapter, we work with the model written down in [2], which is a description of a 3-d Topological insulator adjacent to a superconductor.

3.0.1 Model

The band gaps of topological insulators are much larger than the superconducting gap of all weak-coupling s-wave superconductors. For the purpose of studying the proximity effect between suchsuperconductors and topological insulators, it is sufficient to describe the topological insulator by using the low-energy effective $\vec{k}\cdot\vec{p}$ Hamiltonian. For example, in Bi_2Se_3, this looks like

$$\mathcal{H} = \epsilon(\vec{p}) + A\,\vec{p}\cdot\vec{\alpha} + (M - B\,\vec{p}\cdot\vec{p})\beta - \mu$$

where $\vec{\alpha} = \begin{pmatrix} 0 & \vec{\sigma} \\ \vec{\sigma} & 0 \end{pmatrix}$ and $\beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}_{4\times4}$, an usual 3-d Dirac equation. Since $\epsilon(\vec{p})$ only slightly modifies the curvature, it can be (and from now on is) neglected.

With $M, B > 0$, we see that the spinor has the form $\begin{pmatrix} \Psi_{1\uparrow} \\ \Psi_{1\downarrow} \\ \Psi_{2\uparrow} \\ \Psi_{2\downarrow} \end{pmatrix}$, where 1,2 are hole and particle degrees of freedom respectively. We consider a junction between a metal and a Ti at $z = 0$. To describe metal we put A=0 and make A≠0 for Ti. Moreover, we want the conduction band of the metal aligned with gap of topological insulator, to study how surface states, specifically, change the properties of superconducting state.

Therefore, A(z) and $\mu(z)$ are given by

$$A = A\Theta(z)\mu(z) = E_f\Theta(-z) + \mu\Theta(z)$$

where μ is chemical potential (near the gap) on the TI side. The band structure of the system can be seen on the next page.

Following [2], a simple model of metal can be considered by switching off A in the 3dTI model.

$$H_M = diag[M(\vec{k}), M(\vec{k}), -M(\vec{k}), -M(\vec{k})]$$

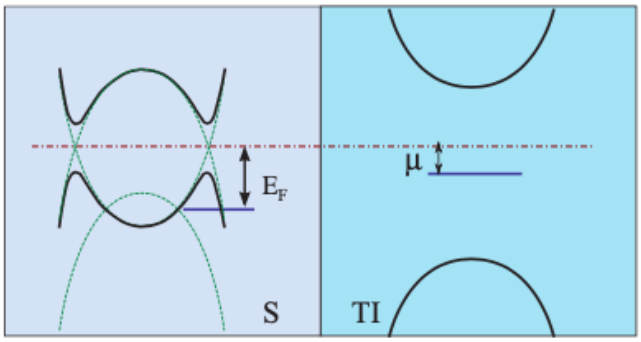

Figure 3.1: Schematic of Metal- TI junction. Taken from [2]

with pairing in conduction band given by

$$H_{int} = \sum_{\vec{\mathbf{k}}} \Delta \cdot \psi^{\dagger}_{2\uparrow}(\vec{\mathbf{k}})\psi^{\dagger}_{2\downarrow}(-\vec{\mathbf{k}}) + h.c.$$

where the order parameter is defined by

$$\Delta\left(z\right) = g\left(z\right)\left\langle \psi_{2\uparrow}\left(\vec{\mathbf{r}}\right)\psi_{2\downarrow}\left(\vec{\mathbf{r}}\right)\right\rangle = g\left(z\right)\int dk_{||}\langle\psi_{2\uparrow}\left(k_{||},z\right)\psi_{2\downarrow}\left(-k_{||},z\right)\rangle$$

where we assume that the system is homegeneous along x,y direction ,Δ is a pure function of z and pairing is only in metal i.e. $g(z) = g\ \Theta(-z)$.

The net hamiltonian of the system is

$$\begin{aligned}\mathcal{H} = \int d\mathbf{k}_{\|}dz \Bigg\{ & \sum_{\sigma}\psi^{\dagger}_{1\sigma}\left(\mathbf{k}_{\|},z\right)\left[h_0 - \mu(z)\right]\psi^{\dagger}_{1\sigma}\left(\mathbf{k}_{\|},z\right) - \sum_{\sigma}\psi^{\dagger}_{2\sigma}\left(\mathbf{k}_{\|},z\right)\left[h_0 + \mu(z)\right]\psi^{\dagger}_{2\sigma}\left(\mathbf{k}_{\|},z\right) \\ & + \Delta(z)\psi^{\dagger}_{2\uparrow}\left(\mathbf{k}_{\|},z\right)\psi^{\dagger}_{2\downarrow}\left(-\mathbf{k}_{\|},z\right) + \text{ H.c.} \\ & + A(z)\left[\psi^{\dagger}_{1\uparrow}\left(-i\partial_z\right)\psi_{2\uparrow} + \psi^{\dagger}_{1\downarrow}\left(i\partial_z\right)\psi_{2\downarrow} + \text{ H.c. }\right] + A(z)\left[\psi^{\dagger}_{1\uparrow}k_{-}\psi_{2\downarrow} + \psi^{\dagger}_{1\downarrow}k_{+}\psi_{2\uparrow} + \text{ H.c. }\right]\end{aligned}$$

where $h_0(\vec{\mathbf{k}}_{||},z) = M - B\partial_z^2 - Bk_{||}^2$.

As in standard BCS, we diagonalize the net system with a bogoliubov transformation, given by

$$\psi_{l\sigma}\left(\mathbf{k}_{\|},z\right) = \sum_{n} u_{n,l\sigma}\left(\mathbf{k}_{\|},z\right)\gamma_{n,\mathbf{k}_{\|}} + v^{*}_{n,l\sigma}\left(\mathbf{k}_{\|},z\right)\gamma^{\dagger}_{n,\mathbf{k}\|}\psi_{l\sigma}\left(\mathbf{k}_{\|},z\right)$$

which will diagonalize the the hamiltonian as

$$H = E_g + \int dk_{||}\sum_{n}\epsilon_n(k_{||})\gamma^{\dagger}_{n,k_{||}}\gamma_{n,k_{||}}$$

where E_g is the ground state energy and γ operators are bogoliubov quasiparticle operators. Functions u and v satisfy

$$\hat{H}_B\Phi(k_{||},z) = \epsilon(k_{||})\Phi(k_{||},z)$$

where the BdG hamiltonian is given by

$$\hat{H}_{BdG} = \begin{pmatrix} h_0 - \mu & \mathbf{d}\cdot\sigma & 0 & 0 \\ \mathbf{d}\cdot\boldsymbol{\sigma} & -h_0 - \mu & 0 & -\Delta i\sigma_y \\ 0 & 0 & \mu - h_0 & \mathbf{d}\cdot\sigma^* \\ 0 & \Delta^* i\sigma_y & \mathbf{d}\cdot\sigma^* & \mu + h_0 \end{pmatrix} \tag{3.1}$$

where wavefunction is a 8×1 spinor given by

$$\Phi = (u_{n,1\uparrow}, u_{n,1\downarrow}, u_{n,2\uparrow}, u_{n,2\downarrow}, v_{n,1\uparrow}, v_{n,1\downarrow}, v_{n,2\uparrow}, v_{n,2\downarrow})$$

and vector $\vec{\mathbf{d}}$ is given by

$$d_x = A(z)k_x,\ d_y = A(z)k_y,\ d_z = A(z) - i\partial_z$$

The self consistency equation in terms of u's and v's is given by like

$$\Delta(z) = g\,(z) \int dk_{11} \sum_{\eta}^{1} u_{n,2\uparrow}\,(k_{11}, z)\, v_{\eta,2\downarrow}\,(-k_{11}, z)\,.\tanh\left(\beta\frac{E_n}{2}\right)$$

3.0.2 Linearization of Self-consistency equation: Computing the Kernel

Following de Gennes's idea, to obtain T_c, we linearize the self consistency equation, by putting u's and v's explicitly from solving the BdG hamiltonian treating Δ as a perturbation.
We rewrite the BdG hamiltonian as

$$H_{BdG} = \begin{pmatrix} H_{AB} & \Delta \\ -\Delta^* & -UH^*_{AB}U\dagger \end{pmatrix}_{8\times 8}$$

where H_{AB} is the net non-interacting system hamiltonain (i.e. metal on LHS, and TI on RHS i.e. simply set $\Delta = 0$ in 3.1). U is given by

$$U = \begin{pmatrix} \sigma_y & 0 \\ 0 & \sigma_y \end{pmatrix}_{4\times 4}$$

Let's call the u_n as the 4×1 spinor denoting the 1st 4 entries of Φ. Similary call the last 4 entries of Φ as v_n. Then u_n and v_n satisfy

$$H_0 u_\eta + \Delta v_\eta = E_n u_n \tag{3.2}$$
$$-UH_0^* U^t v_n - \Delta^* u_n = E_n v_n \tag{3.3}$$

Now expand u's and v's in orders of Δ as

$$u_n = u_n^0 + u_n^1 + u_n^2 + \ldots \tag{3.4}$$
$$v_n = v_n^0 + v_n' + v_n^2 + \ldots \tag{3.5}$$

with 1st order corrections taken to be

$$u_n^1 = \sum e_{\eta m} u_m^0 \tag{3.6}$$

$$v_n^1 = \sum d_{nm} v_m^0 \tag{3.7}$$

Now if $H_{AB}\phi_n = \xi_n \phi_n$ then $u_n^0 = \phi_n$ if $\xi_n > 0$ and $v_n = U\phi_n^*$ if $\xi_n < 0$.
Then we have

$$\left(H_0 u_n^0 + H_0 u_n^1\right) + \Delta\left(v_n^0\right) = E_n^0 u_n + E_n^0 u_n^1 \tag{3.8}$$

$$\Rightarrow E_n^0 u_n^1 - H_0 u_n^1 = \Delta v_n^0 \tag{3.9}$$

$$\Rightarrow \left(E_n^0 - \xi_m\right) e_{nm}\phi_n = \Delta v_n^0 \tag{3.10}$$

$$\Rightarrow e_{nm} = \int \frac{\phi_m^\dagger \Delta v_n^0 d\overrightarrow{r}}{E_n^0 - \xi_m} \tag{3.11}$$

which can worked out to yield

$$e_{nm} = \int d\overrightarrow{r}\Delta\left(\overrightarrow{r}\right) \times (-i) \times \frac{\left[\phi_{m2\uparrow}^*\left(\overrightarrow{r}\right)\phi_{n2\uparrow}^*\left(\overrightarrow{r}\right) + \phi_{m2\downarrow}^*\left(\overrightarrow{r}\right)\phi_{n2\downarrow}^*\left(\overrightarrow{r}\right)\right]}{E_n^0 - \xi_m}$$

Similarly we find

$$d_{nm} = \int d\overrightarrow{r}\Delta^*\left(\overrightarrow{r}\right) \times (i) \times \frac{\left[\phi_{m2\uparrow}\phi_{n2\uparrow} + \phi_{m2\downarrow}\phi_{n2\downarrow}\right]}{E_n^0 - \xi_m}$$

With coefficients e's and d's calculated, we can plug it back into self consistency equation to get

$$\Delta(s) = g\left(s\right) \int dk_{11} \sum_n{}' u_{n2\uparrow}^{(1)}\left(k_{11}, z\right) v_{\eta 2\downarrow}^{*0}\left(-k_{11}, z\right) + u_{\eta 2\uparrow}^0\left(k_{11}, z\right) v_{\eta 2\downarrow}^{1*}\left(-k_{11}, z\right)$$

Now the idea is to put the 1st order corrections from above equations. They involve coefficients e and d, which in turn involve Δ. Therefore, the RHS will involve an integral of Δ. Theregfore, the final result will be of the form

$$\Delta(z) = \int K(z, w) \cdot \Delta(w)\, dw$$

where K is the linearized kernel. Now we write the form of the kernel

$$K(\vec{\mathbf{s}}, \vec{\mathbf{r}}) = 2k_B T \sum_\omega \Big[\ G_{\uparrow\uparrow}^\omega(\vec{\mathbf{s}}, \vec{\mathbf{r}}) \cdot G_{\uparrow\uparrow}^{-\omega}(\vec{\mathbf{s}}, \vec{\mathbf{r}}) + G_{\uparrow\downarrow}^\omega(\vec{\mathbf{s}}, \vec{\mathbf{r}}) \cdot G_{\uparrow\downarrow}^{-\omega}(\vec{\mathbf{s}}, \vec{\mathbf{r}}) + G_{\downarrow\downarrow}^\omega(\vec{\mathbf{s}}, \vec{\mathbf{r}}) \cdot G_{\downarrow\downarrow}^{-\omega}(\vec{\mathbf{s}}, \vec{\mathbf{r}})\ \Big] \tag{3.12}$$

where

$$G_{\alpha,\beta}^\omega(x, x') = \sum_i \frac{\phi_{i,2\alpha}(x, x')\phi_{i,2\beta}^*(x, x')}{\xi_i - i\omega} \tag{3.13}$$

where α, β are spin indices, $\phi_{i,2\alpha}$ is the wavefunction of the non-interacting problem of metal - Ti junction placed adjacently corresponding to the i^{th} eigenstate. Important to note that only $|\xi| < \omega_D$ need to be summed to compute the effective green's functions G^ω.

Chapter 4

Discussion and Future Scope

The kernel derived in previous chapter can be computed analytically and the profile of pair potential, consequently, sovled. However, we've realized that there are 2 bottlenecks in this process:

- One needs to solve for wavefunctions ϕ by usual rules of standard quantum mechanics: Match ϕ and its derivatives at the boundary. Though straightforward, the leads to 8 equations, which are non-linear in $k_z, k_{||}$, which renders computing effective green's function tedious. We've tried to get around this by working with the effective hamiltonian near fermi surface, where pairing is predominantly present. However, this needs to be done with a bit of caution as the matching problem is non-trivial. For example, one needs to allow for the possibility that even if an electron from the conduction band is incident on the interface (with e^{ikx} as it's travelling solution), it can reflect as a hole in the valence band with a decaying $e^{-\beta x}$ profile. This make sense as for the valence band, the electron is above it's band, so travelling solutions aren't possible.

- Even if one does solve for the kernel (which we did, albeit some approximations), this is still a self-consistent equation i.e. LHS and RHS depend on each other. Therefore, we cannot simply solve it without making further accommodations. One of the typical ways is to assume a step function profile of the pairing potential (present only on the metal side) and then solve by plugging it again and again toarrive at the actual $\Delta(z)$ in an order by order series type of fashion. Although deGennes bypassed this problem as he could find a differential equation for the kernel K, here, since K has non-translational invariance built into it's arguments, a similar idea is difficult to concoct.

If one uses the method highlighted in second point, one needs to continually solve for pair potential and set it to 0 to get T_c. this would mean that one has T_c perturbatively, instead of arriving at it in one shot. However, it seems since $\Delta(x > 0)^{-lambdax}$, where λ is the decay length for surface state, it could be the case that self-consistent equation can be simplified, by only taking values of Δ withing $\frac{1}{\lambda}$ length of TI while calculating changes to T_c. We are trying to simplify this calculation to predict T_c or atleast provide some boudns on it.

Appendix A

Derivation of Linearized Self-Consistency equation for near T_c analysis

A.0.1 Δ as a perturbation

(This section has been taken from de Gennes chapter 7)

We start with eqn (1.0.2) determining the self-consistency

$$\Delta(\vec{r}) = V(r) \sum_n v_n^*(\vec{\mathbf{r}}) u_n(\vec{\mathbf{r}})\ tanh(\beta E_n/2)$$

where u_n, v_n are positive eigenvalues of the BdG equations (1.5) given by

$$\begin{pmatrix} H_0(\vec{\mathbf{r}}) & \Delta(\vec{\mathbf{r}}) \\ \Delta^*(\vec{\mathbf{r}}) & -H_0^*(\vec{\mathbf{r}}) \end{pmatrix} \begin{pmatrix} u_n(\vec{\mathbf{r}}) \\ v_n(\vec{\mathbf{r}}) \end{pmatrix} = \epsilon_n \begin{pmatrix} u_n(\vec{\mathbf{r}}) \\ v_n(\vec{\mathbf{r}}) \end{pmatrix} \tag{A.1}$$

We expand the above equation as a power series in Δ by expanding u, v order by order in Δ

$$u_n = u_n^0 + u_n^1 + \ldots v_n = v_n^0 + v_n^1 + \ldots$$

Now plugging this back in, we see that u_n^0, v_n^0 is propotional to eigenfunctions ϕ_n defined by the eqn

$$\xi_n \phi_n = \left[\frac{(\hat{\vec{\mathbf{p}}} - q\vec{\mathbf{A}})^2}{2m} + U(r) - \mu \right] \phi_n$$

To zeroth order we have

$$u_n^0 = \phi_n, v_n^0 = 0 \qquad (\xi_n > 0) u_n^0 = 0, v_n^0 = \phi_n^* \qquad (\xi_n < 0)$$

which gives excitation energies $\epsilon_n = |\xi_n|$. This makes $u_n^0 v_n^{(0)*} = 0$, so plugging this back into (1.0.2) won't give any corrections. Now we go for first order corrections

$$u_n^1 = \sum_m e_{nm} \phi_m v_n^1 = \sum_m d_{nm} \phi_m^*$$

Plugging this into (A.0.1), mutliplying ϕ_m^* in the first, ϕ_m in the second and integrating, we find

$$(|\xi_n| - \xi_m) e_{nm} = \int \Delta(r) \phi_m^*(r) v_n^0(r) d\vec{\mathbf{r}} (|\xi_n| + \xi_m) d_{nm} = \int \Delta^*(r) \phi_m(r) u_n^0(r) d\vec{\mathbf{r}}$$

Here we've set $e_{nn} = 0$ to preserve the normalization of $\begin{pmatrix} u_n(\vec{\mathbf{r}}) \\ v_n(\vec{\mathbf{r}}) \end{pmatrix}$. An easy way to check is that if we set $\Delta = 0$, we should end up with a normalised spinor. Moreover, normalization is important since the value of $\Delta(r)$ depends on it (but the exciation energies don't).

Now we can, once again, use these and plug them back (1.0.2) to get

$$\Delta(\vec{r}) = V(r) \sum_n \left(v_n^{(0)*}(\vec{\mathbf{r}}) u_n^1(\vec{\mathbf{r}}) + v_n^{1,*}(\vec{\mathbf{r}}) u_n^0(\vec{\mathbf{r}}) \right) tanh(\beta|\xi|_n/2)$$

Simplifying this and using the fact that $v_n^{(0)}(\vec{\mathbf{r}}) = 0, \ for \ |\xi_n| > 0$ and with a similar consideration for u_n^0 , along with the fact that tanh(x) is odd in x, we get

$$\Delta(s) = \int K(s,r)\Delta(r)dr$$
$$K(s,r) = \frac{V}{2} \sum_{nm} \frac{tanh(\beta\xi_n/2) + tanh(\beta\xi_m/2)}{\xi_n + \xi_m} \times \quad \phi_n^*(r)\phi_m^*(r)\phi_n(s)\phi_m(s)$$

Using the fact that $tanh(\frac{\beta\xi}{2}) = 2k_BT \sum_\omega \frac{1}{\xi - i\hbar\omega}$, where ω are odd fermionic masturbara frequencies (both +ve and -ve), this further simplified to

$$K(s,r) = Vk_BT \sum_\omega \sum_{nm} \frac{\phi_n^*(\vec{\mathbf{r}})\phi_m^*(\vec{\mathbf{r}})\phi_n(\vec{\mathbf{s}})\phi_m(\vec{\mathbf{s}})}{(\xi_n - i\hbar\omega)(\xi_m + i\hbar\omega)}$$

In the paper, is just inner part without the frequency sum in the above equation. This result is advantageous for the following reasons:

- We've eliminated u, v and instead replaced them with the familiar one-electron wavefunctions ϕ_m - The only unknown left is $\Delta \implies$ no additional complexity of solving the BdG equations for new u,v from a given Δ (in some sense the Kernel accounts for them)

However, the only caution to be taken is that this would work near T_c, where the linearized form holds.

For the case of $\vec{\mathbf{B}}$ incident on the sample, this kernel needs some modification. de Gennes section titled "Separation of Magnetic effects" clearly discusses these effects. I mention one key takeaway from that section:

- On Validity of kernel : It is shown that the integral equation (A.0.1) is valid for normal metals near T_c. Turns out, for dirty metals, it gets better and one can replace at **all temperatures** the linear integral equation by a second order differential equation of Landau ginzburg form (more on this later)

A.0.2 Impurities, Averaging and Translational Invariance

Consider the kernel $K(\vec{\mathbf{s}}, \vec{\mathbf{r}})$ in an infinite homogenous medium. If the system is a pure metal, then it's clear that it's a function of $\vec{\mathbf{s}} - \vec{\mathbf{r}}$. However, for an alloy (i.e. by alloy de Gennes means a metal with some impurities), this is property is **precluded**. One way to restore translational invariance is to average over the impurity configurations. Then the RHS of (A.0.1) becomes $\overline{K(\vec{\mathbf{s}}, \vec{\mathbf{r}})\Delta(\vec{\mathbf{r}})}$ which can then be approximated as $\overline{K(\vec{\mathbf{s}}, \vec{\mathbf{r}})\Delta(\vec{\mathbf{r}})} \to \overline{K(\vec{\mathbf{s}}, \vec{\mathbf{r}})} \cdot \overline{\Delta}(\vec{\mathbf{r}})$. This approximation isn't strictly rigorous as it neglects

distortion of pair potential in immediate neighbourhood of impurity, but nonetheless has been shown to be reasonable. Then the idea is to employ the kernel eqn(A.0.1) but with averaged $\overline{\Delta(r)}$ instead of actual, now with the fact that impurity averaged $\overline{K(\vec{\mathbf{s}},\vec{\mathbf{r}})}$ is just a function of $\vec{\mathbf{s}}-\vec{\mathbf{r}}$.

A.0.3 Relation between K_0 and a Correlation Function

Simple relations in case of Infinite Homogenous mediums (Clean + Dirty)

Note: $K(\vec{\mathbf{s}},\vec{\mathbf{r}})$ is henceforth referred to as K_0 (de Gennes differentiates b/w both in case of$\vec{\mathbf{A}}\neq 0$, however that's impertinent for our T_c calculations. We shall treat them as the same thing).

The appearance of four wavefunctions in (A.0.1) seems a little artificial. However, one can represent the kernel in terms of a more physical quantity, a correlation function, which is immediately known in many cases, making this connection particularly useful. For simplicity, first we start with a **infinite homogenous** medium, and do a fourier transform of $K(\vec{\mathbf{s}},\vec{\mathbf{r}})$ to get

$$\begin{aligned} K(\vec{\mathbf{q}}) &= L^{-3}\int d\vec{\mathbf{r}}d\vec{\mathbf{s}}K_0(\vec{\mathbf{s}}-\vec{\mathbf{r}})e^{i\vec{\mathbf{q}}\cdot(\vec{\mathbf{s}}-\vec{\mathbf{r}})} \\ &= VL^{-3}k_BT\sum_{\omega,n,m}\frac{\langle n|e^{iqs}|m\rangle\cdot\langle m|e^{-iqr}|n\rangle}{(\xi_n-i\hbar\omega)(\xi_m+i\hbar\omega)} \end{aligned}$$

where L^{-3} is the volume of solid.

the 1st e^{iqx} is corresponding to e^{iqs} while the second corresponds to e^{-iqr}. However, the fourier transform here assumes translational invariance.

"Admonitory Note: This invariance isn't available to us in in-homogenous situations, however we can get around it"

Let's take $\vec{\mathbf{q}}$ along x- direction. Then the matrix elements referred above means

$$\langle n|e^{i\vec{\mathbf{q}}\vec{\mathbf{x}}}|m\rangle = \int w_n(\vec{\mathbf{r}})e^{i\vec{\mathbf{q}}\cdot\vec{\mathbf{r}}}w_m(\vec{\mathbf{r}})d\vec{\mathbf{r}}$$

Now consider the real function

$$\begin{aligned} g(\vec{\mathbf{q}},\Omega) &= \sum_m \overline{\langle n|e^{iqx}|m\rangle\ \langle m|e^{-iqx}|n\rangle}\delta(\xi_m-\xi_n-\Omega) \\ &= \sum_m \overline{\left|\langle n|e^{iqr}|m\rangle\right|^2}\,\delta(\xi_m-\xi_n-\Omega) \end{aligned}$$

where we average over all states of **fixed energy** ξ_n (for example $\xi_n=0$ represents fermi level) i.e. an avg over all such $|n\rangle$ with same energy. In avg, $g(\vec{\mathbf{q}},\Omega)$ depends strongly on Ω but only slightly on ξ_n. Now supposing we know $g(\vec{\mathbf{q}},\Omega)$, we can calculate $K_0(\vec{\mathbf{q}})$ as

$$\begin{aligned} K_0(\vec{\mathbf{q}}) &= VL^{-3}k_BT\sum_{\omega,n,m}\frac{\langle n|e^{iqx}|m\rangle\cdot\langle m|e^{-iqx}|n\rangle}{(\xi_n-i\hbar\omega)(\xi_m+i\hbar\omega)} \\ &= N(0)Vk_BT\sum_{\omega}\int\frac{d\xi' d\xi\quad g(\vec{\mathbf{q}},\frac{\xi'-\xi}{\hbar})}{(\xi-i\hbar\omega)(\xi'+i\hbar\omega)} \end{aligned}$$

In the above we've put back the implicit assumption that the works only in a thing ring around Fermi surface in the ξ integration (hence $N(0)$, the dos at Fermi energy. ¡font size=4, color='red'¿¡b¿Where did another $N(0)$ go?¡/b¿¡/font¿). Moreover, this naturally dictates the energy ξ_n states $|n\rangle$ in (A.0.3), namely that we've to average over states at the fermi level i.e. $\xi_n = 0$. This a important point to keep in mind: ξ_n sums are cutoff at ω_d as in BCS (where ξ_n is just ξ_k).

Let's introduce the Heisenberg operator to write

$$e^{i\vec{\mathbf{q}}\cdot\vec{\mathbf{x}}(t)} = exp(i\hat{\mathcal{H}}_0 t)e^{iqx}exp(-i\hat{\mathcal{H}}_0 t)$$

which describes the evolution of $exp(iq\hat{x})$ in time for an electron in the pure metal subjected to $\hat{\mathcal{H}}_0 = p^2/2m + U(r)$. In terms of this operator, $e^{iqx(t)}$, $g(\vec{\mathbf{q}}, \Omega)$ looks like

$$\begin{aligned} g(\vec{\mathbf{q}}, \Omega) &= \sum_m \overline{\langle n|e^{iqs}|m\rangle\ \langle m|e^{-iqr}|n\rangle}\delta(\xi_m - \xi_n - \hbar\Omega) \\ &= \sum_m \int \frac{dt}{2\pi}\, exp(-i(\xi_m - \xi_n - \hbar\Omega)t)\, \overline{\langle n|e^{iqs(t)}|m\rangle\ \langle m|e^{-iqr}|n\rangle} \cdot\ exp(i(\xi_m - \xi_n)) \\ &= \int \frac{dt}{2\pi\hbar}\, e^{i\Omega t}\, \overline{\langle n|e^{iqs(t)}\ e^{-iqr}|n\rangle} \end{aligned}$$

Therefore, in order to determine g, one only need determine the correlation function for e^{iqx}

$$\langle e^{-iqx}e^{iqx(t)}\rangle_{E_F} = \overline{\langle n|e^{iqx(t)}\ e^{-iqx}|n\rangle}$$

for an electron at Fermi energy in a normal metal, where we assume that $x(0) = r$ and $x(t) = s$. This is quite a simplification.

1. For normal metal: Since for free particle we know that $\hat{x}(t), \hat{p}(t)$ evolve mathematically in the same way as in classical mechanics (Ehrenfest theorem), we can replace $\hat{x}(t) = x_0 + v_F t\ \cdot cos(\theta)$ (v_F because we want to average on fermi sphere), where v_F cos(θ) is the x-component of velocity, (since q is in x-direction). Then the avg yields

$$\begin{aligned} \langle e^{-iqx(0)}e^{iqx(t)}\rangle_{E_F} &= \frac{1}{4\pi}\int d\phi\ sin(\theta)d\theta\ exp(iqv_F \cdot cos(\theta)t) \\ \implies g(\vec{\mathbf{q}}, \Omega) &= \frac{1}{2\hbar}\int_0^\pi sin\theta d\theta\ \delta(\Omega - qv_F cos(\theta)) \\ &= \begin{cases} (2qv_F\hbar)^{-1} & |\Omega| < qv_F \\ 0 & |\Omega| > qv_F \end{cases} \end{aligned}$$

2. For dirty metals: For impure metals, $x(t)$ is controlled by a diffusion process, in lieu of scattering from various impurities. Therefore, we calculate the $e^{iqx(t)}$ correlation using classical ideas of drift-diffusion equation, which, for a particle starting at $x(t = 0) = x_0$, gives the probability $P(x, t)$ of the particle being subsequently present at x at time t as

$$P(x,t) = \frac{1}{\sqrt{4\pi Dt}}e^{-\frac{(x-x_0)^2}{4Dt}}$$

where D is the diffusion constant. Now we've two lengthscales in this situation:

- l, the mean free path of the electron in the metal - q^{-1} coming from e^{iqx}, which provides a characteristic wavlength of spatial variation

Now suppose, $l \gg q^{-1}$. This means when taking the average $\langle e^{-iqx(0)}e^{iqx(t)}\rangle$, we have a fast oscillating 2nd term, whose average shall be small. Alternatively, one can think that we're trying to avergage the wavefunction of a free-particle at two different times. If the free particle has oscillated much farther than the length q^{-1} i.e. on a scale comparable with that from quantum considerations (e^{iqx} is afterall a free particle), we can no longer just claim that the process is controlled just by diffusion. Constrast this with the opposite limit viz. $l \ll q^{-1}$. This means that the particles oscillates on a much smaller scale than it's quantum-given-wavelength, and this small scale oscillation is accounted for by diffusion. Therefore, we can get away by doing a standard classical average, instead of doing a full quantum average (which, given that there are impurities, will not be as simple).

Therefore, averaging the correlation $\langle e^{-iqx(0)}e^{iqx(t)}\rangle$ using the correlation above

$$\begin{aligned}\langle e^{-iqx(0)}e^{iqx(t)}\rangle_F &= \int_{-\infty}^{\infty} dx\ e^{iq(x-x_0)}\ \frac{1}{\sqrt{4\pi Dt}} e^{-\frac{(x-x_0)^2}{4Dt}} \\ &= \sqrt{\pi}\ e^{-q^2 D|t|} \qquad ql \ll 1\end{aligned}$$

Note that we've simply used diffusion equation and not drift-diffusion equation (which might be a tempation given we're averaging over fermi surface which allows for a typical speed v_F, so it might be tempting to use this v_F as drift velocity). This would unphysical as it would imply that there is some background wind flowing at v_F that drifts our electron.

Also, we take diff. coefficient as $D = v_F l/3$ (i'm not sure why the 3 appears here, but otherwise given what we know of diffusion coefficient, it generally has the form $(\delta x)^2/(\delta t)$, where we assume that the particle hops δx distance in time δt with a certain hopping probability. Now, since the correlation is being averaged over fermi-surface, we can see $\delta x/\delta t \sim v_F$ and $\delta x \to l$. The latter is easy to see from the derivation of discretized drift-diffusion equation, where the particle hops to a site spaced δx from origin and then probabilistically hops to another such site (much like electron in a metal colliding after traversing l distance). And given that our electron sits on fermi-surface, it's natural to assume that it does such hopping at a rate v_F).

Calculating $g(\vec{\mathbf{q}}, \Omega)$ from this (using (A.0.3)) we've

$$g(\vec{\mathbf{q}}, \Omega) = \frac{1}{\pi\hbar}\frac{Dq^2}{\Omega^2 + D^2q^4} = \frac{1}{2\pi\hbar}\left\{\frac{1}{i\Omega + Dq^2} + h.c.\right\} \qquad ql \ll 1$$

A.0.4 Explicit Calculation of the kernel K_0

Using the forms of $g(\vec{\mathbf{q}}, \Omega)$ derived above, we can determine $K_0(\vec{\mathbf{q}})$. We take the variable of integration as $\xi, \hbar\Omega = \xi' - \xi$.

1. For pure metal First ξ integral is performed via residues to get

$$\begin{aligned}K_0(\vec{\mathbf{q}}) &= \frac{N(0)Vk_BT}{qv_F\hbar}\sum_{\omega}\int_{-qv_F}^{qv_F}\frac{d\Omega}{2\omega - i\Omega} \\ &= \frac{2\pi N(0)Vk_BT\pi}{qv_F\hbar}\sum_{\omega} tan^{-1}(\frac{qv_F}{2|\omega|})\end{aligned}$$

2. For dirty metals

$$K_0(\vec{\mathbf{q}}) = N(0)Vk_bT\frac{2i}{\hbar}\sum_{\omega}\int d\Omega\frac{Dq^2}{(Dq^2+i\Omega)\cdot(2i\omega+\Omega)}$$
$$= \frac{N(0)Vk_BT}{\hbar}\sum_{\omega}\frac{1}{Dq^2+2|\omega|} \qquad (ql \ll 1)$$

A.0.5 Some comments on the above results

- We see that nowhere ω_D comes up in the calculation of the kernel, which should've been the case since V couples only those states ξ, ξ' with satisfy $|\xi|, |\xi'| < \hbar\omega_D$. This is then reflected in divergence for $q = 0$ mode (in both cases). One way to remedy this to explicitly calculate $K_0(q = 0)$ and set

$$K_0(\vec{\mathbf{q}}) = K_0(\vec{\mathbf{q}} = 0) + \{K_0(\vec{\mathbf{q}}) - K_0(\vec{\mathbf{q}} = 0)\}$$

The divergent $K_0(\vec{\mathbf{q}} = 0)$ piece is found calculated as

$$K_0(\vec{\mathbf{q}} = 0) = L^{-3}\int d\vec{\mathbf{r}}\, d\vec{\mathbf{s}}\, K_0(\vec{\mathbf{s}} - \vec{\mathbf{r}})$$
$$= V\sum_n \frac{tanh(\frac{\beta\xi_n}{2})}{2\xi_n}$$
$$\xrightarrow[Cutoff\ scale\ (-\omega_D,\omega_D)]{Now\ we\ cut\ the\ energy\ integral} \frac{V}{2}\int_{-\omega_d}^{\omega_D}\frac{d\xi}{2\xi}tanh(\frac{\beta\xi}{2}) = N(0)V\ ln\left(\frac{1.14\hbar\omega_D}{k_BT}\right)$$

For homogenous case, demanding a spatially constant pairing potential means that $K_0(\vec{\mathbf{q}} = 0) = 1$. This can then used to find critical temperature (or more generally, the highest temperature at which a non-zero root is possible for pairing potential is defined as critical temperature).

For a exact spatial dependence, an inverse fourier transform reveals:

- For pure metal:

$$K_0(\vec{\mathbf{s}}, \vec{\mathbf{r}}) = K_0(\vec{\mathbf{R}}) = \frac{N(0)Vk_bT}{2\hbar v_F}\sum_{\omega}\frac{1}{R^2}\cdot exp(-2\frac{|\omega|R}{v_F})$$

  where R is $s - r$. For large $|R|$, only the lowest matsubara frequency $\omega_0 = \pm\pi k_BT \sim \pm\pi k_BT_c$ is important, which leads to

$$K(R) \sim exp(-2\pi\frac{R}{(\frac{\hbar v_F}{k_BT_c})}) \sim exp(-1.13R/\xi_0)$$

  where $\xi_0 = 0.18\frac{\hbar v_F}{k_BT_c}$ which is nearly same as superconducting coherence length in BCS theory.

- For a dirty metal

$$K_0(R) = \frac{N(0)Vk_BT}{2\hbar D}\sum_{\omega}\frac{1}{R}exp(-\sqrt{\frac{2|\omega|}{D}}R) \qquad (R \gg l)$$

The $R \gg l$ emerges from $ql \ll 1$. It might be also resonable to think of the pure metal as a dirty metal with huge l, the pure metal answer forms the $R \ll l$ part of the above result. We see now the corresponding ξ_{dirty} from the exponential is read off as (again as we consider the large R and $\omega = \pm\pi k_B T_c$ limit)

$$\xi_{dirty} \sim \sqrt{\xi_0 \times l}$$

All this works for $R \gg l$ limit , which transforms as $\xi_{dirty} \gg l \implies \xi_0 \gg l$. When this is satisfied, for an alloy (or any medium for that matter), it is termed as "dirty".

Comment: We can see that a small mean free path reduces ξ. Hence one can expect that impurities might change a type-I SC (low λ/ξ) to type 2 SC (high λ/ξ) just by adding impurities. This has been experimentally verified for various impurities in indium (see de Gennes foot note on pg 224)

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