

Aspects of superconductivity and fractionalization

by

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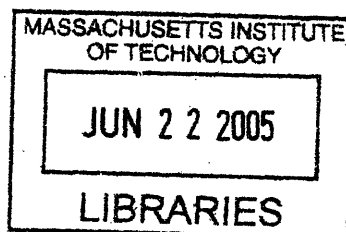
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Abstract

Since their discovery in mid 80's, a complete theory of high temperature superconductors is yet to take its final shape. Theory of fractionalization attempts to explain the phenomenon by assuming that the electron is split into two particles, chargin and spinon, carrying charge and spin respectively. Although capable of producing the qualitative features of the phase diagram, this theory is not been able to account for a number of experimental observations. A simple mean field model based on fractionalization ideas is proposed in this work which can possibly get around some of the drawbacks of the original fractionalization theory. Chapter one discusses various aspects of superconductivity along with BCS theory and chapter two talks about the motivation behind considering this model along with its basic features.

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Contents

1 Superconductivity	11
1.1 Superconductivity phenomenon	11
1.1.1 Zero resistivity	12
1.1.2 Meissner effect	12
1.1.3 Isotope effect	14
1.1.4 Electronic specific heat	14
1.2 BCS Theory	15
1.2.1 Cooper pairs and origin of attractive interaction	15
1.2.2 The BCS Hamiltonian	16
1.2.3 Gap equation and excitation spectrum	17
1.2.4 Comparison of BCS predictions against experiments	19
1.3 High Temperature Superconductivity	21
2 Fractionalization and the mean field model	25
2.1 Fractionalization	25
2.2 Motivation	26
2.2.1 Problems with fractionalization	26
2.2.2 Possible solution	27
2.3 The simplified mean field Hamiltonian	28
2.4 Conclusion	29

List of Figures

1-1	Resistivity as a function of temperature	12
1-2	Meissner effect for type I superconductors	13
1-3	Meissner effect for type II superconductors	14
1-4	Behaviour of electronic specific heat with temperature	15
1-5	Electron interaction via phonon exchange	16
1-6	High T_c superconductor phase diagram	23
2-1	Phase diagram for the modified Hamiltonian	27
2-2	RVB configuration [4]	30

Chapter 1

Superconductivity

Superconductivity is one of the greatest discoveries in physics during the course of twentieth century. Apart from showing zero resistance, superconducting state has also shown some very peculiar physical properties. Even after its discovery, by Kammerlingh Onnes in 1911, a complete theory of conventional superconductivity didn't appear till mid 50's when Bardeen, Cooper and Schrieffer [1] gave a thorough account of various superconductivity phenomenon. This theory is popularly known as BCS theory and it demonstrated superconductivity as a truly quantum mechanical phenomenon. A brief account of conventional superconductivity and BCS theory is given in sections one and two respectively. Since its discovery by Bednorz and Müller in 1986, high temperature (high T_c) superconductivity has remained one of the most active and competitive research areas in physics. Section three discusses various properties of high T_c superconductors and failure of BCS theory to account for the phenomenon.

1.1 Superconductivity phenomenon

In this section a brief account of important properties of superconductors are given. Such peculiar characteristic properties shown by all conventional superconductors were instrumental in directing the ideas for developing a theoretical description of the phenomenon.

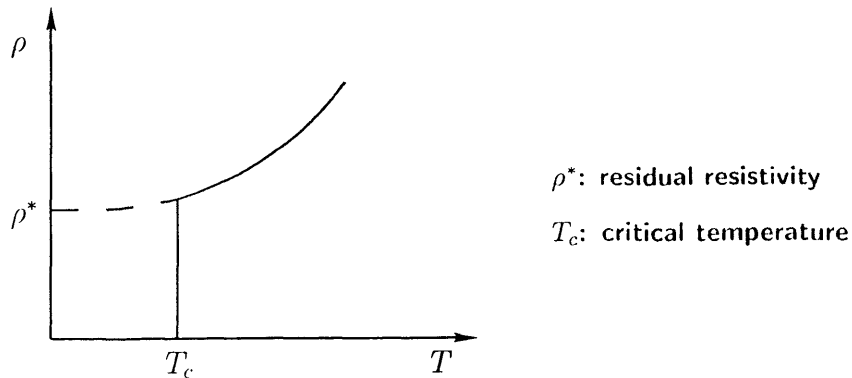


Figure 1-1: Resistivity as a function of temperature

1.1.1 Zero resistivity

One of the most striking characteristics of Superconductors is their non-existent resistivity below a certain critical temperature, T_c . Certain experiments have shown that the currents in superconducting circuits continue to persist months or years from the time they are first put into the material. It appears as though these materials are carrying currents with a very practical hundred percent efficiency. The low critical temperatures have prevented the widespread use of superconductors in many industrial applications that can benefit from this efficiency.

1.1.2 Meissner effect

It was discovered in 1933 by Meissner and Ochsenfeld that a superconductor will expel magnetic flux from its interior acting like a perfect diamagnet. In fact, based on Maxwell's equations one can calculate the depth to which magnetic flux can penetrate in simple metals. It is called London penetration depth, λ_L is inversely related to superfluid density and is of the order of hundreds of Angstroms for conventional superconductor and thousands of Angstroms for high temperature superconductors.

$$\frac{1}{\lambda_L^2} = \frac{4\pi n_s e^2}{mc^2}. \quad (1.1)$$

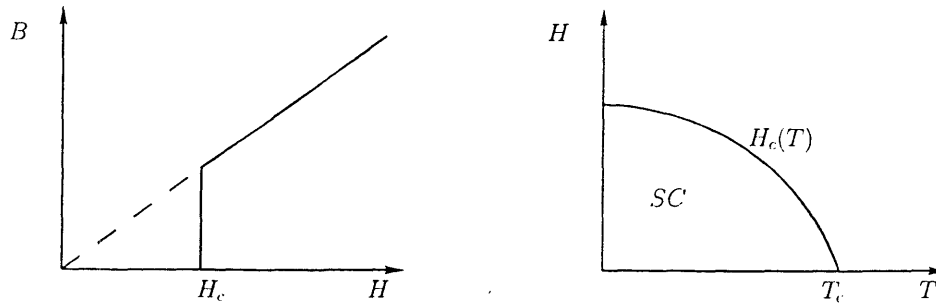


Figure 1-2: Meissner effect for type I superconductors

Simple explanation for this effect is that the impinging magnetic field will coerce eddy currents that oppose the magnetic field, and since the material has zero resistivity, these eddy currents will persist and will continue to repulse the magnetic field, even after it has stopped changing. Thus a superconductor behaves as a perfect diamagnet. If the field gets too large, say more than H_c , the material will eventually lose its superconducting state as there wouldn't be enough superconducting electrons to sustain these currents. Although, this explains perfect diamagnetism based on perfect conduction, it doesn't convey the complete physics related to Meissner effect. If a sample is cooled in external magnetic field, the magnetic field would be expelled from the interior once the sample becomes superconducting. Thus Meissner effect can be considered as an independent property of superconductors in addition to the property of perfect conduction. There were two types of superconducting materials, called type I and type II which responded differently to external magnetic fields. For type I, magnetic field is completely shielded from the interior of the superconductors. For type II, magnetic field is partially shielded in the interior of a superconductor. For type II superconductors, the magnetic field in the superconductor is concentrated along flux tubes when the applied magnetic field lies between two critical values, H_{c1} and H_{c2} .

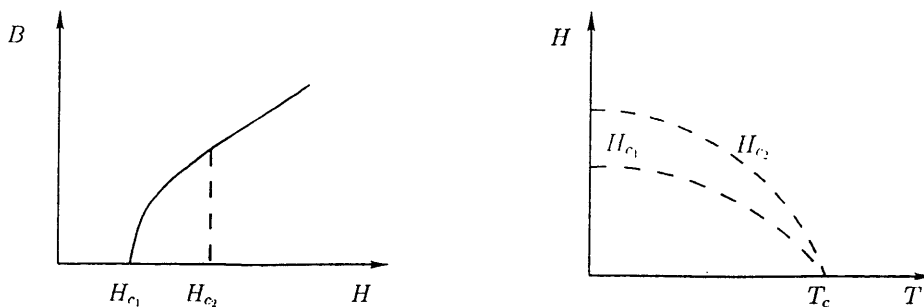


Figure 1-3: Meissner effect for type II superconductors

1.1.3 Isotope effect

For various elements, the superconducting transition temperature T_c was observed to be different for different isotopes. Since neutrons carry no charge, they do not affect the coulombic interactions between electrons and lattice ions, but they do change the rates at which phonons can propagate through the lattice. A phonon is a mechanical wave, and it is one of the fundamental parts of the BCS theory. BCS theory can accurately predict how these isotope effects arise in simple metal superconductors.

1.1.4 Electronic specific heat

There are several thermodynamic changes that occur in a superconductor as it makes its transition from the normal region ($T > T_c$) to the superconducting region ($T < T_c$). The specific heat capacity of an electron changes from a linear relationship with temperature to an exponential relationship. The plot of specific heat with temperature suggests a second-order phase transition that increases the specific heat about three times as temperature is decreased to below T_c . The exponential decay in the specific heat of the form $c = e^{-\Delta/k_B T}$, with Δ of the order of $k_B T_c$, indicated that there is a gap in the excitation spectrum which was later confirmed through experiments. The singularity in specific heat at T_c indicated presence of a phase transition.

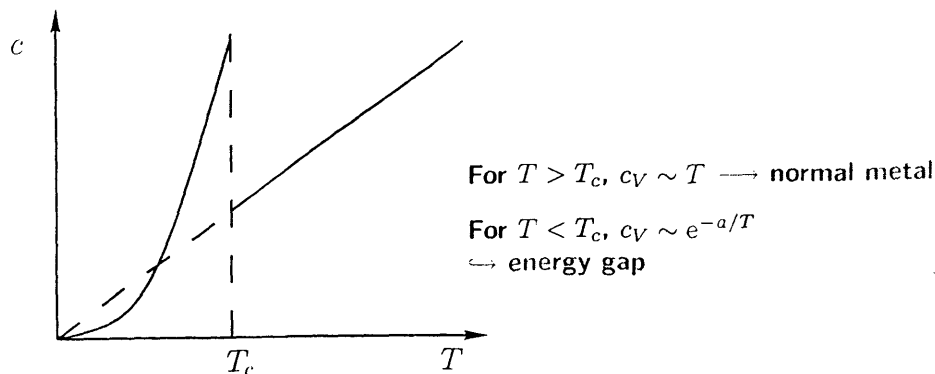


Figure 1-4: Behaviour of electronic specific heat with temperature

1.2 BCS Theory

As discussed in previous section, the exponential decay of electronic specific heat indicated the presence of a gap in the excitation spectrum. A band gap would have also accounted for zero resistance. If charge carriers can move through a crystal lattice without interacting at all, it must be because their energies are quantized such that they do not have any available energy levels that they can occupy after scattering from ions. Further study of absorption spectrum for electromagnetic radiation revealed that the absorption occurs only when the energy $\hbar\omega$ of incident photon is greater than about 2Δ . This clearly suggested that the excitations giving exponential behaviour to specific heat are created in pairs. Isotope effect suggested that the superconducting transition involved some kind of interaction with the crystal lattice. All these observations together indicated that theory of superconductivity should take into account interaction between a pair of electrons through phonon exchange.

1.2.1 Cooper pairs and origin of attractive interaction

One of the most important ingredients of the microscopic theory of superconductivity is that the electrons close to the Fermi surface can be bound in pairs by an attractive interaction forming Cooper pairs. Since there is no cost in free energy for adding or subtracting a fermion at the Fermi surface, a condensation phenomenon can take

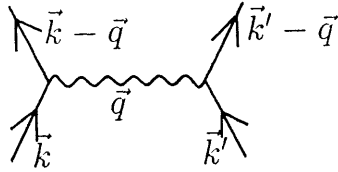


Figure 1-5: Electron interaction via phonon exchange

place if two fermions are bounded by energy E_B , lowering the energy of the system by the same amount. Therefore we get more stability by adding more and more bounded pairs at the Fermi surface. Any pair of electrons would repel due to coulomb interaction and hence the attractive potential should be large enough to outweigh this repulsion. Phonons, quanta of lattice vibrations, interact with electrons and can give rise to attractive potential. An electron attracts the positive ions in its vicinity to itself, and this higher density of positive charge can overscreen the coulombic repulsion between the electrons and can cause attraction between electrons. If the temperature is too large, the number of random phonons in the lattice due to thermal processes will destroy this coupling and hence destroy the superconductivity at high temperatures.

1.2.2 The BCS Hamiltonian

After understanding that the phenomenon involved phonon interaction a simplified Hamiltonian could be constructed which could address the problem. Consider Feynman diagram of two electrons scattering off each other by phonon mediation : If H_0 is the Hamiltonian representing free electrons and phonons then the effective Hamiltonian of system of electrons interacting through transfer of phonons is given by,

$$H = H_0 + \sum_{\mathbf{k}, \mathbf{s}, \mathbf{k}', \mathbf{s}', \mathbf{q}} W_{\mathbf{k}, \mathbf{k}', \mathbf{q}} c_{\mathbf{k}'+\mathbf{q}, \mathbf{s}'}^\dagger c_{\mathbf{k}-\mathbf{q}, \mathbf{s}}^\dagger c_{\mathbf{k}, \mathbf{s}} c_{\mathbf{k}', \mathbf{s}'} \quad (1.2)$$

The matrix element, $W_{\mathbf{k},\mathbf{k}',\mathbf{q}}$, representing the phonon interaction is of the form,

$$W_{\mathbf{k},\mathbf{k}',\mathbf{q}} = \frac{|M_{\mathbf{q}}|^2 \hbar \omega_{\mathbf{q}}}{(\xi_{\mathbf{k}} - \xi_{\mathbf{k}-\mathbf{q}})^2 - (\hbar \omega_{\mathbf{q}})^2}. \quad (1.3)$$

Now, one can consider the superconducting electron system as being in some sort of a condensate phase with electrons with opposite spin and momentum forming a pair. Thus only the interaction between such a pair would be considered in estimating the energy of the system. With this assumption, the ground state can lower its energy by considerable amount as compared to unperturbed Fermi liquid state. The BCS Hamiltonian for electrons with this assumption and including Coulomb repulsion is given by,

$$H_{BCS} = \sum_{\mathbf{k}} \xi_{\mathbf{k}} (c_{\mathbf{k}\uparrow}^\dagger c_{\mathbf{k}\uparrow} c_{-\mathbf{k}\downarrow}^\dagger c_{-\mathbf{k}\downarrow}) - \sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}'\downarrow}^\dagger c_{-\mathbf{k}\downarrow} c_{\mathbf{k}'\uparrow}. \quad (1.4)$$

Where $\xi_{\mathbf{k}} = \epsilon_{\mathbf{k}} - \mu$ with $\epsilon_{\mathbf{k}}$ is energy of the free electron and μ is fermi energy (which is same as chemical potential at low temperatures) and $V_{\mathbf{k},\mathbf{k}'}$ which includes screened Coulomb repulsion $U_{\mathbf{k},\mathbf{k}'}$ is given by

$$V_{\mathbf{k},\mathbf{k}'} = -2W_{-\mathbf{k},\mathbf{k}',\mathbf{k}'-\mathbf{k}} - U_{\mathbf{k},\mathbf{k}'} \quad (1.5)$$

1.2.3 Gap equation and excitation spectrum

Once the simplified Hamiltonian is obtained, the next step is to find the expression for quasiparticle excitation energies which should indicate the presence of a gap. One can diagonalize such a Hamiltonian with quartic interaction by using the Bogoliubov-Valatin transformation with quasi particle operators, $\gamma_{\mathbf{k}}$ and $\gamma_{-\mathbf{k}}$.

$$\gamma_{\mathbf{k}} = u_{\mathbf{k}} c_{\mathbf{k}\uparrow} - v_{\mathbf{k}} c_{-\mathbf{k}\downarrow}^\dagger \quad \gamma_{-\mathbf{k}} = u_{\mathbf{k}} c_{-\mathbf{k}\downarrow} + v_{\mathbf{k}} c_{\mathbf{k}\uparrow}^\dagger \quad (1.6)$$

These operators satisfy fermionic anti-commutation relations with $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ being real numbers and $u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2 = 1$. One can write the BCS Hamiltonian in terms of quasiparticle operators and elimination of the off-diagonal terms which would give a Hamiltonian of system of independent fermions. The condition for vanishing of

off-diagonal terms can be written as

$$2\xi_{\mathbf{k}}u_{\mathbf{k}}v_{\mathbf{k}} - (u_{\mathbf{k}}^2 - v_{\mathbf{k}}^2) \sum_{\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} u_{\mathbf{k}'} v_{\mathbf{k}'} = 0 \quad (1.7)$$

By defining $\Delta_{\mathbf{k}} = \sum_{\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} u_{\mathbf{k}'} v_{\mathbf{k}'}$ and using $u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2 = 1$ one can arrive at the integral equation for the gap parameter $\Delta_{\mathbf{k}}$ given by

$$\Delta_{\mathbf{k}} = \frac{1}{2} \sum_{\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} \frac{\Delta_{\mathbf{k}'}}{(\xi_{\mathbf{k}'}^2 + \Delta_{\mathbf{k}'}^2)^{1/2}} \quad (1.8)$$

Above equation is called 'gap equation'. After eliminating the off diagonal interaction terms, one gets a Hamiltonian which is given by,

$$H_{BCS} = E_N + \sum_{\mathbf{k}'} E_{\mathbf{k}}(m_{\mathbf{k}} + m_{-\mathbf{k}}). \quad (1.9)$$

Here, $m_{\mathbf{k}} = \gamma_{\mathbf{k}}^\dagger \gamma_{\mathbf{k}}$ and $m_{-\mathbf{k}} = \gamma_{-\mathbf{k}}^\dagger \gamma_{-\mathbf{k}}$ denote the number operators for excitations. E_N is the ground state energy and $E_{\mathbf{k}}$ is the energy of elementary excitations and these two are given by

$$E_N = \sum_{\mathbf{k}} 2\xi_{\mathbf{k}}v_{\mathbf{k}}^2 - \sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} u_{\mathbf{k}}v_{\mathbf{k}}u_{\mathbf{k}'}v_{\mathbf{k}'} \quad (1.10)$$

$$E_{\mathbf{k}} = (\xi_{\mathbf{k}}^2 + \Delta_{\mathbf{k}}^2)^{1/2} \quad (1.11)$$

Ground state is annihilated by both gamma operators and is given by

$$|\Psi_0\rangle = \left[\prod_{\mathbf{k}} (u_{\mathbf{k}} + v_{\mathbf{k}} c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger) \right] |0\rangle \quad (1.12)$$

At finite temperatures, for calculating physical quantities, the $m_{\mathbf{k}}$ operators can be replaced by their thermal averages, namely by Fermi-Dirac distribution function. Due to nonzero value of quasi-particle excitations, the gap parameter decreased as temperature increases and eventually goes to zero at a critical temperature T_c .

1.2.4 Comparison of BCS predictions against experiments

Once the excitation spectrum is known one can go on to calculate various physical quantities and check for consistency with the experiment. For simplicity one can consider a model for potential $V_{\mathbf{k}\mathbf{k}'}$.

$$\begin{aligned} V_{\mathbf{k}\mathbf{k}'} &= V && \text{if } \xi_{\mathbf{k}} < \hbar\omega_D \\ &= 0 && \text{otherwise} \end{aligned}$$

Here V is a constant and $\hbar\omega_D$ is Debye energy. In this assumption, $\Delta_{\mathbf{k}}$ is constant too and can be calculated by explicit integration. The final expression is given by [3]

$$\Delta = \frac{\hbar\omega_D}{\sinh[1/VD(\mu)]} \quad (1.13)$$

Where $D(\mu)$ is density of states at Fermi energy. One can estimate the product $VD(\mu)$ by noting that,

$$V \sim \frac{|M_{\mathbf{q}}|^2}{\hbar\omega_D} \quad (1.14)$$

Electron-phonon interaction amplitude $|M_{\mathbf{q}}|$ can be given from Fröhlich Hamiltonian by [3]

$$\begin{aligned} |M_{\mathbf{q}}| &\sim \sqrt{\frac{N\hbar k_F^2}{M\omega_D}} |V_{\mathbf{k}}| \\ \Rightarrow |M_{\mathbf{q}}| &\sim \frac{Nm\mu}{M\hbar\omega_D} |V_{\mathbf{k}}|^2 \end{aligned}$$

Where $V_{\mathbf{k}}$ is Fourier transform of screened ion potential. Since $D(\mu) \sim N/\mu$ one finds that

$$VD(\mu) \sim \frac{m}{M} \left(\frac{NV_{\mathbf{k}}}{\hbar\omega_D} \right)^2 \quad (1.15)$$

While $\hbar\omega_D$ is of the order of 0.03 eV, the factor $NV_{\mathbf{k}}$ which is average screened ion potential over the unit cell, is around few electron volts. Thus $(NV_{\mathbf{k}}/\hbar\omega_D)^2$ is of the

order of 10^4 . m/M is the ration of electron mass to ion mass and is around 10^{-5} . Under these approximations, $VD(\mu)$ is of the order of .1 and hence one can replace \sinh in expression for Δ by exponential function. Thus,

$$\Delta = 2\hbar\omega_D e^{-1/VD(\mu)} \quad (1.16)$$

is a very small quantity, about one percent of the Debye energy and hence corresponds to a temperature of the order of 1K. If the electron phonon interaction is too strong then this approximation is not valid and one can get a bigger value for Δ . But, one can see that the superconducting transition temperatures predicted by BCS theory are very low temperatures, much lower than those corresponding to high T_c superconductors.

To get finite temperature effects one replace the quasiparticle number operators by thermal averages for fermions (i.e. Fermi-Dirac function). Thus,

$$\bar{m}_{\mathbf{k}} = \bar{m}_{-\mathbf{k}} = f(E_{\mathbf{k}}) = \frac{1}{\exp(E_{\mathbf{k}}/k_B T) + 1} \quad (1.17)$$

This modifies the gap equation to :

$$\Delta_{\mathbf{k}}(T) = \frac{1}{2} \sum_{\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} \frac{\Delta_{\mathbf{k}'}(T)}{[\xi_{\mathbf{k}'}^2 + \Delta_{\mathbf{k}'}^2(T)]^{1/2}} [1 - 2f(E_{\mathbf{k}'})] \quad (1.18)$$

By considering same assumption as before for $V_{\mathbf{k}\mathbf{k}'}$ and by understanding that the gap vanished at T_c , one arrives at following expression for transition temperature :

$$k_B T_c = 1.14\hbar\omega_D e^{-1/VD(\mu)} \quad (1.19)$$

This along with the value for zero temperature gap gives $2\Delta_0/k_B T_c = 3.5$ which is in good agreement with experiments which give value lying between 2 and for 5 for most elements. Isotope effect is evident from expression for T_c as it involves the Debye frequency which is proportional to square root of ionic mass. By considering the thermal averages one can also get the expression for the energy of the system and

hence specific heat. In the simple model considered for $V_{\mathbf{k}\mathbf{k}'}$, one can see that the specific heat is given by :

$$c(T) = \sum_{\mathbf{k}} \left(\frac{d\Delta^2}{dT} - \frac{2E_{\mathbf{k}}^2}{T} \right) \frac{\partial f}{\partial E_{\mathbf{k}}} \quad (1.20)$$

The observed discontinuity in specific heat arises from the derivative term as Δ is not smooth across T_c . The equation predicts a increase by a factor of 2.5 in specific heat, as the element is cooled through T_c , which is in reasonable agreement with experiments.

Thus we can see that the BCS theory can indeed account for various observed phenomenon regarding conventional superconductors. High T_c superconductors exhibit a number of peculiar properties that cannot be explained within BCS theory and that is the topic of discussion for the next section.

1.3 High Temperature Superconductivity

All conventional superconductors had an upper cutoff critical temperatures of around $30^\circ K$ which was what BCS theory suggested. One can increase T_c by making the lattice more rigid, and thereby increasing ω_D , the cutoff frequency for electron phonon interaction. But this would at the same time decrease the electron-phonon interaction. Another way of increasing T_c would be increasing the density of electron states near fermi energy, thereby making the ground state more stable. But, due to electron-phonon interaction, the phonon spends part of its time as a virtual electron-hole pair. Thus increasing the electron density beyond certain limit results in decreasing the effective frequency of the phonons and hence critical temperature T_c . It was a pleasant surprise when, in 1986, Bednorz and Müller discovered that superconductivity occurred at 35K in certain compound of lanthanum, barium, copper and oxygen.

High temperature superconductivity is exhibited by only a particular class of materials, the rare earth copper oxides with various kinds of dopants. They are layered materials consisting of copper oxide(CuO_2) planes in which the copper atoms

form a square lattice and oxygen atoms lie between each nearest-neighbor pair of copper atoms. The rest of the atoms, rare earth atoms, dopants and excess copper and oxygen form charge reservoir layers separating the square planar CuO_2 layers. These charge reservoir layers influence the oxidation state of the planar copper atoms, which is either Cu^{++} or Cu^{+++} . The parent undoped compound is an insulator and has all the planar coppers atoms in the Cu^{++} state, with one unpaired spin per site. In a systems which has an average density of one electron per site, the conduction is suppressed by large Coulomb energy required for double occupation. Such a collective Coulomb blockade makes the undoped compound an insulator. The unpaired electron spins order anti-ferromagnetically, so that neighboring spins are anti-parallel. The resulting state is called a Mott insulator. High temperature superconductivity occurs when the undoped parent compound is doped with holes. Removing electrons or equivalently adding holes to these materials both destabilizes the anti-ferromagnetic spin order and relieves the electronic congestion, turning them from insulators to conductors.

High T_c materials are often described in terms of a phase diagram having temperature (T) and doping (x) as two axes, where x is the number of excess holes per planar copper atom. Such a phase diagram is shown in the figure. The solid lines in this figure denote phase boundaries. For low doping, the compound is in anti-ferromagnetic phase denoted by A. The maximum temperature for which this order persists happens for $x=0$. The transition temperature for this phase falls off rapidly with increasing x and appears to fall to zero for x of a few per cent. For larger values of x , there is another phase boundary, containing the superconducting phase, S. This phase has its maximum transition temperature at what is called optimal doping. To the left of this point, materials are said to be underdoped, and to the right they are overdoped.

In addition to sharp phase boundaries there is also a well-defined crossover line to a pseudogap phase. For underdoped materials, gap -like features appear at temperatures much higher than the superconducting T_c giving a pseudo-gap phase. This is not a sharp transition, and so the bold dashed curve in figure simply indicates the tem-

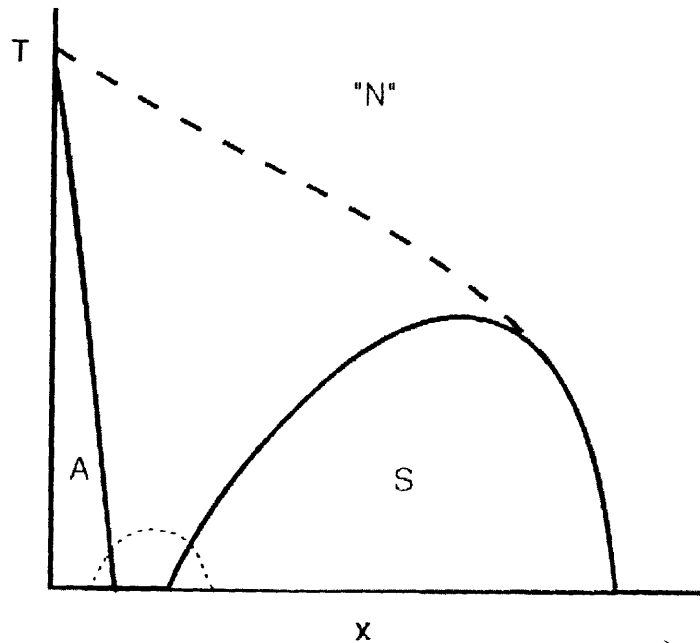


Figure 1-6: High T_c superconductor phase diagram

peratures below which the existence of this pseudogap becomes evident. Finally there is a part of the phase diagram at low temperatures, indicated by the thin dashed line, overlapping the region where anti-ferromagnetism disappears and superconductivity grows up, where the system may exhibit a variety of phases. In this region there is evidence for spin glass behavior and for charge-modulated mesophases called stripes. It is even possible for the charge and doping to be modulated from layer to layer - a phenomenon called staging. For different high T_c compounds, different behaviors are observed in this region of the phase diagram. It appears that, in the vicinity of the crossover from anti-ferromagnetism to superconductivity, there are many competing phases that can be stabilized by small variations in the chemistry. As a result, this region is poorly understood.

While BCS state for conventional superconductivity was obtained as a perturbation to the Fermi liquid state, the parent undoped compound for high T_c superconductors is Mott insulator. The anomalous normal-state properties of the cuprates clearly suggest that these materials are not just a normal Fermi liquid above T_c , and therefore may not be adequately described by BCS theory below T_c . The electrical

dc resistivity $\rho(T)$, exhibits a linear dependence in temperature over a wide range of temperatures above T_c . For a conventional Fermi liquid associated with normal metals, $\rho(T) \sim T^2$. This is a manifestation of the long lifetime of electrons near the Fermi surface in a conventional Fermi liquid. The nuclear spin-lattice relaxation rate $T_1^{-1}(T)$ shows a temperature dependence substantially different from that of normal metals. Other anomalous normal-state properties of the copper-oxide superconductors include the thermal conductivity $\kappa(T)$, the optical conductivity $\sigma(\omega)$, the Raman scattering intensity $S(\omega)$, the tunneling conductance as a function of voltage $g(V)$, and the Hall coefficient $R_H(T)$. All of these normal-state properties are quite uncharacteristic of the Fermi liquid usually associated with the normal state of conventional superconductors.

Early experimental studies usually assumed that the superconductivity was s-wave and interpreted all of the data in terms of that assumption. After clear demonstration of the linear temperature dependence of the low T penetration depth, possibility that the superconducting gap might have nodes and d-wave symmetry was taken very seriously. In a d-wave superconductor, quasiparticles near the nodes can be excited at low temperatures thereby causing a steeper decrease in superfluid density. A superconducting pairing state with $d_{x^2-y^2}$ symmetry has the energy gap of the form: $\Delta(\vec{k}, T) = \Delta_o(T) | \cos(k_x a) - \cos(k_y a) |$. where $\Delta_o(T)$ is the maximum value of the energy gap at temperature T and a is the lattice constant or distance between nearest neighbor Cu atoms in the plane. The angular momentum and spin of a Cooper pair is L=2 and S=0, respectively (i.e. singlet $d_{x^2-y^2}$ pairing).

All these aspects clearly suggest high T_c superconductivity to be a quite different phenomenon not explained by BCS theory. Among various options explored, fractionization ideas have contributed significantly, towards a complete theory of high T_c superconductivity. Next chapter talks about this in the context of Z_2 gauge theory.

Chapter 2

Fractionalization and the mean field model

In this chapter a simplified model based on fractionalization ideas would be presented. The first section talks about basic idea behind Z_2 gauge theory of fractionalization. In section two motivation behind the new model is given and third section discusses basic features of the model. In the end a short conclusion is given talking about the scope of the model for further work.

2.1 Fractionalization

Strongly interacting many-electron systems in low dimensions can exhibit exotic properties, for example : the presence of excitations with fractional quantum numbers. In these cases, the electron is ‘fractionalized’, i.e. effectively broken into the constituents which essentially behave as free particles. The basic constituents being, chargon and spinon carrying charge and spin of the electron respectively. The classic example of this splitting is the one-dimensional (1d) interacting electron gas. Electron ‘fractionalization’ is also predicted to occur in 2d systems in very strong magnetic fields that exhibit the fractional quantum Hall effect. It is believed that this idea of fractionalization of the electron could occur under conditions that are far less restrictive than the two examples mentioned above. Once the electron is fractionalized, it’s charge

is no longer tied to its Fermi statistics. The resulting charged boson (the chargon) can then directly condense leading to superconductivity. There is a third distinct excitation, namely, the flux of the Z_2 gauge field (dubbed the vison). Vison is gapped in fractionalization phase.

2.2 Motivation

2.2.1 Problems with fractionalization

The Z_2 gauge theory of fractionalization had several drawbacks in terms of explaining the observed properties of high T_c superconductors. One of the observed features of cuprates is linear decreasing of superfluid density, ($n_s(T)$), with low temperatures. The slope of this decrement is observed to be independent of doping x . Thus $n_s(T) = n_s(0) - AT$ with $n_s(0) \sim x$ but A independent of x . In fractionalization theory, $n_s(0) \sim x$ is obeyed but, as the current carried by nodal quasi-particle is proportional to doping, the coefficient A is proportional to x^2 .

As mentioned in the previous section, the Z_2 gauge theory implies existence of a gapped excitation; the Z_2 vortex or "vison". Visions are the topological defects occurring in the underlying order of Z_2 gauge field and hence are believed to have excitation energy of the order of interbond interaction. However, experiments of detecting vison have led to negative results, putting bounds on vison gap to be less than 200K which is an order of magnitude less than the natural scale $J \sim 1000K$.

Another inconsistency of the theory with experiments was regarding spectral functions obtained using ARPES. Fractionalization predicted that the nodal spectral function doesn't change drastically as temperature decreases below T_c while the antinodal spectral function shows sharp excitations as temperature decreases below T_c . Behaviour of nodal spectral function is inconsistent with the experiments.

Another feature of cuprates is their small magnetoresistance in pseudo-gap region showing metallic behaviour. In conventional superconductors, just above T_c , thermodynamic fluctuations produce small, transient regions of the superconducting state,

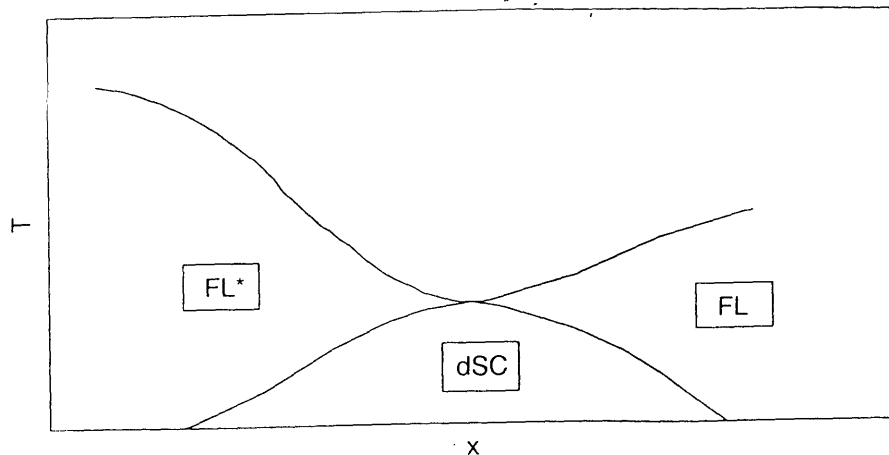


Figure 2-1: Phase diagram for the modified Hamiltonian

giving rise to an anomalous increase in the normal-state conductivity. Within the framework of fractionalization, the transport in pseudo-gap region which is because of charge motion would probably be analogous to that of a superconductor near critical region giving large magnetoresistance. Fractionalization also proposed an fractionalized antiferromagnetic state for doping close to zero. The antiferromagnetic order in such states would not get destroyed quickly on doping. Experimentally, it is observed that the antiferromagnetic order persists for a relatively small doping.

2.2.2 Possible solution

One can possibly get around some of the inconsistencies of the theory through certain modifications. Assume that the pseudo-gap state as a fractionalized fermi liquid phase (denoted by FL^*). Doped holes are assumed to form a Fermi surface of volume x which consists of four small pockets centered at $(\pm\pi/2, \pm\pi/2)$. Holes behave as elementary excitations at this Fermi surface and co-exist with d-wave paired spinons. Spinons and holes have average number given by $\langle f^\dagger f \rangle = 1$ and $\langle c^\dagger c = x \rangle$ respectively. Transition to superconducting phase (denoted by dSC) would happen when $\langle c^\dagger f \rangle \neq 0$. Based on these assumptions one expects the model to have qualitative features indicated in the diagram. In the underdoped dSC phase one expects to have quasi particle excitations with current of $O(1)$ which would make coefficient A independent of doping. One also expects the hole pockets centered

around nodal points along $k_x = k_y$ to give metallic behaviour to charge transport and hence giving low magnetoresistance. In FL^* Quasiparticle excitations along $k_x = k_y$ would be sharp and would be expected not to change significantly across T_c . In this model, presence of spinful fermionic holes carrying charge-e would disturb the magnetic order making AF^* phase fall sharply with doping. More work might be needed to get around the difficulty associated with flux-trapping experiments.

2.3 The simplified mean field Hamiltonian

The Hamiltonian for the model is given by :

$$H = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k},c} c_{\mathbf{k},\sigma}^\dagger c_{\mathbf{k},\sigma} + \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k},f} f_{\mathbf{k},\sigma}^\dagger f_{\mathbf{k},\sigma} + \sum_{\mathbf{k}} \Delta_{\mathbf{k}} \left(f_{\mathbf{k},\uparrow}^\dagger f_{-\mathbf{k},\downarrow}^\dagger + f_{-\mathbf{k},\downarrow} f_{\mathbf{k},\uparrow} \right) + b \sum_{\mathbf{k},\sigma} \left(c_{\mathbf{k},\sigma}^\dagger f_{\mathbf{k},\sigma} + f_{\mathbf{k},\sigma}^\dagger c_{\mathbf{k},\sigma} \right) \quad (2.1)$$

Here the coupling b is zero in FL^* phase (which occurs above T_c) and is not equal to zero in dSC. Further b is assumed to be function of temperature with $b(0) \sim \sqrt{x}$. $\Delta_{\mathbf{k}}$ denotes $d_{x^2-y^2}$ pairing. To diagonalize the Hamiltonian, define,

$$d_{\mathbf{k},\uparrow} = f_{\mathbf{k},\uparrow}, d_{\mathbf{k},\downarrow} = f_{-\mathbf{k},\downarrow}^\dagger, h_{\mathbf{k},\uparrow} = c_{\mathbf{k},\uparrow}, h_{\mathbf{k},\downarrow} = c_{-\mathbf{k},\downarrow}^\dagger. \quad (2.2)$$

$$\Rightarrow H = \sum_{\mathbf{k}} \epsilon_{\mathbf{k},c} h_{\mathbf{k}}^\dagger \sigma^z h_{\mathbf{k}} + \sum_{\mathbf{k}} d_{\mathbf{k}}^\dagger (\epsilon_{\mathbf{k},f} \sigma^z + \Delta_{\mathbf{k}} \sigma^x) d_{\mathbf{k}} + b \sum_{\mathbf{k}} \left(h_{\mathbf{k}}^\dagger \sigma^z d_{\mathbf{k}} + d_{\mathbf{k}}^\dagger \sigma^z h_{\mathbf{k}} \right) \quad (2.3)$$

Let,

$$\Psi_{\mathbf{k}} = \begin{pmatrix} h_{\mathbf{k}} \\ d_{\mathbf{k}} \end{pmatrix} \quad (2.4)$$

$$\Rightarrow H = \sum_{\mathbf{k}} \Psi_{\mathbf{k}}^\dagger M_{\mathbf{k}} \Psi_{\mathbf{k}} \quad (2.5)$$

Where,

$$M_{\mathbf{k}} = \begin{pmatrix} \epsilon_{\mathbf{k},c} & 0 & b & 0 \\ 0 & -\epsilon_{\mathbf{k},c} & 0 & -b \\ b & 0 & \epsilon_{\mathbf{k},f} & \Delta_{\mathbf{k}} \\ 0 & -b & \Delta_{\mathbf{k}} & -\epsilon_{\mathbf{k},f} \end{pmatrix} \quad (2.6)$$

Quasiparticle excitation energies are eigenvalues of $M_{\mathbf{k}}$ given by:

$$2\xi_{\mathbf{k}}^2 = \epsilon_{\mathbf{k},c}^2 + E_{\mathbf{k}}^2 + 2b^2 \pm \sqrt{(\epsilon_{\mathbf{k},c}^2 - E_{\mathbf{k}}^2)^2 + 4b^2(\epsilon_{\mathbf{k},c}^2 + E_{\mathbf{k}}^2 + 2\epsilon_{\mathbf{k},c}\epsilon_{\mathbf{k},f})} \quad (2.7)$$

Where,

$$E_{\mathbf{k}}^2 = \Delta_{\mathbf{k}}^2 + \epsilon_{\mathbf{k},f}^2 \quad (2.8)$$

Location of gapless excitations would be given by $\det M_{\mathbf{k}} = 0$ which can be found as follow :

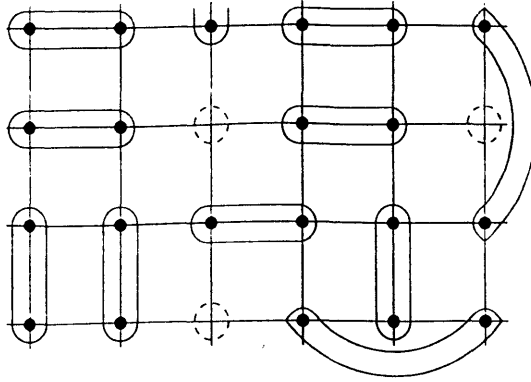
$$\begin{aligned} \Rightarrow \det M_{\mathbf{k}} &= 0 \\ \Rightarrow \epsilon_{\mathbf{k},c}^2 E_{\mathbf{k}}^2 - 2b^2 \epsilon_{\mathbf{k},c} \epsilon_{\mathbf{k},f} - b^4 &= 0 \\ \Rightarrow (\epsilon_{\mathbf{k},c} \epsilon_{\mathbf{k},f} - b^2)^2 + \epsilon_{\mathbf{k},c}^2 \Delta_{\mathbf{k}}^2 &= 0 \end{aligned}$$

Thus at the quasiparticle nodes one must have : $\Delta_{\mathbf{k}} = 0$ and $\epsilon_{\mathbf{k},c} \epsilon_{\mathbf{k},f} - b^2 = 0$. Thus the gapless points are only along the lines $k_x = \pm k_y$ as required by experiments. To solve the second condition one can assume the dispersion relations for hole and spinon as : $\epsilon_{\mathbf{k},c} \approx a(k^2 - k_0^2)$ $\epsilon_{\mathbf{k},f} \approx v_{1f}k$

Here k is the distance along the diagonal from the location of spinon node given by $(\pi/2, \pi/2)$. k_0 , the fermi wave-vector, behaves as $k_0 \sim \sqrt{x}$ for a two dimensional system. The second condition for gapless points can now be written as $k(k^2 - k_0^2) = b^2/av_{1f}$. It is proved in the appendix 1 that such a equation would have only one root for sufficiently small doping x .

2.4 Conclusion

Although a first hand estimate of calculation of superfluid density, done in appendix 2, looks promising, more work is required to determine various other properties of the model. The resonating valence bond (RVB) phenomenon is coming out as a promising candidate for explaining high T_c superconductivity. In an RVB configuration, each electron pairs with another electron to form a singlet bond. An RVB state is



$$r \text{ --- } r' = \frac{|\uparrow_r \downarrow_{r'}\rangle - |\downarrow_r \uparrow_{r'}\rangle}{\sqrt{2}}$$

Figure 2-2: RVB configuration [4]

a superposition of many such configurations, all having same energy. The ground state of doped cuprates is believed to have a significant overlap with the RVB state. The simplified model given, considers spinon interacting with holes with interaction strength dependent on doping. Something very similar happens in an intuitive model of RVB induced superconductivity. Consider an RVB configuration in which there is an isolated pair of unbonded electron (considered as spinon) and hole lying next to each other. One can form another RVB configuration with positions of the two, hole and electron, reversed. These two configurations have same energy and hence an infinitesimal amount of electric field can cause a system existing in one configuration to go to one existing in the other. Result of such an event would be a net flow of charge in the direction of the electric field. A sufficiently large number of such events could give rise to a continuous motion of holes causing superconduction. One also expects more events of electron and hole exchange as doping is increased. Exchange of electrons and holes can only take place along x and y directions, which may induce directional character to the interaction which might be able to account for the d-wave nature of the superconductor. All these observations make the Z_2 gauge theory, along with the model considered, a promising development towards explaining the

high temperature superconductivity.

Appendix 1

Existance of only one gapless point

The cubic equation that we need to consider is given by

$$k(k^2 - k_0^2) = b^2/av_{1f} \quad (2.9)$$

As both k_0 and b have leading doping dependence of \sqrt{x} , the equation can be re-written as:

$$\begin{aligned} k(k^2 - \alpha x) &= \beta x \\ k^3 - \alpha x k - \beta x &= 0 \end{aligned}$$

For an arbitrary x , one can find the number of roots as follow: Let, $f(k) = k^3 - \alpha x k - \beta x$ which would has a minima and maxima at k equal to $\sqrt{\alpha x/3}$ and $-\sqrt{\alpha x/3}$ respectively. As $f(0)$ is less than zero, there can be only one root for $k > 0$. There can be double root on the negative k axis if $f(-\sqrt{\alpha x/3}) > 0$.

$$\begin{aligned} \Rightarrow -\frac{\alpha x}{3} \sqrt{\frac{\alpha x}{3}} + \alpha x \sqrt{\frac{\alpha x}{3}} - \beta x &> 0 \\ \Rightarrow \frac{2\alpha x}{3} \sqrt{\frac{\alpha x}{3}} - \beta x &> 0 \\ \Rightarrow \frac{2}{3\sqrt{3}} \alpha^{3/2} \sqrt{x} &> \beta \end{aligned}$$

Thus, for $x \sim 0$, there would be only one root.

Appendix 2

Calculating physical quantities in the model

Once the Hamiltonian is written in terms of quasiparticle excitations, one can proceed on the lines of BCS calculations to find out various properties expected from the model. Here I would sketch how one can go around doing the calculations. The superfluid density as a function of temperature can be given by :

$$n_s = n_0 - \frac{e^2}{m} \int d^2k k^2 \left(\frac{-\partial f(\xi_{\mathbf{k}})}{\partial \xi_{\mathbf{k}}} \right) \quad (2.10)$$

One gets the same expression in BCS theory and one can use the same tricks to simplify the expression as those used in the theory. For low temperatures, the decrement in the density is determined by the size of quasiparticle excitations around node and is given by

$$n_s = n_0 - mk_B T \frac{k_{node}^2}{v_F v_\phi} \quad (2.11)$$

Here, $v_F = \frac{-\partial \xi_{\mathbf{k}}}{\partial k}$ and $v_\phi = \frac{1}{k} \frac{-\partial \xi_{\mathbf{k}}}{\partial \phi}$ and they parametrize the quasiparticle dispersion in the vicinity of the node. To proceed further into the calculation, one needs to realize that in the earlier calculations k was measured with respect to the spinon node. While in the above formula for superfluid density assumes $k=0$ as the origin of the 2D k space. So we need to shift the origin of the 2D k space to spinon node. If θ is the original polar coordinate which defines $\Delta(\theta) = \Delta_0 \cos(\theta)$ and ϕ is the polar coordinate of a system located at spinon node then, $\delta\theta \sim k\delta\phi$. And so, $v_\phi \sim \frac{\partial \xi_{\mathbf{k}}}{\partial \theta}$. After a bit of labour one can get the two velocities required in terms of energies or wave vector

at quasiparticle node. Calculation of various derivatives is little bit treaky and my approach relies on expanding excitation energy as a Taylor around the node. For calculating v_F , one can simplify the analysis by assuming that Δ is zero. This should be valid as node lies on the $\Delta = 0$ line. I assumed that the $\epsilon_{\mathbf{k},c}$ and $\epsilon_{\mathbf{k},f}$ can be expressed as $\epsilon_{\mathbf{k},c,node} + \delta\epsilon_{\mathbf{k},c}$ and $\epsilon_{\mathbf{k},f,node} + \delta\epsilon_{\mathbf{k},f}$ respectively with $\epsilon_{\mathbf{k},c,node}\epsilon_{\mathbf{k},f,node} = b^2$. After doing the expansion, one gets expression for $\delta\xi_{\mathbf{k}}$ in terms of various quantities at node and $\epsilon_{\mathbf{k},c,node}\epsilon_{\mathbf{k},f,node} = b^2$. One can read off the derivative from this expression,

$$2 \left(\frac{\partial \xi_{\mathbf{k}}}{\partial k} \right)^2 = \left(\epsilon'_{\mathbf{k},c} \epsilon'_{\mathbf{k},f} [a] + \epsilon'^2_{\mathbf{k},c} [b] + \epsilon'^2_{\mathbf{k},f} [c] \right)_{node} \quad (2.12)$$

with,

$$\begin{aligned} [a] &= \left[1 - \left(\frac{\epsilon_{\mathbf{k},c} - \epsilon_{\mathbf{k},f}}{\epsilon_{\mathbf{k},c} + \epsilon_{\mathbf{k},f}} \right)^2 \right] \\ [b] &= \left[\frac{1}{2} + \left(\frac{\epsilon_{\mathbf{k},c} - \epsilon_{\mathbf{k},f}}{\epsilon_{\mathbf{k},c} + \epsilon_{\mathbf{k},f}} \right)^2 - \left(\frac{\epsilon_{\mathbf{k},c} - \epsilon_{\mathbf{k},f}}{\epsilon_{\mathbf{k},c} + \epsilon_{\mathbf{k},f}} \right) \right] \\ [c] &= \left[\frac{1}{2} + \left(\frac{\epsilon_{\mathbf{k},c} - \epsilon_{\mathbf{k},f}}{\epsilon_{\mathbf{k},c} + \epsilon_{\mathbf{k},f}} \right)^2 + \left(\frac{\epsilon_{\mathbf{k},c} - \epsilon_{\mathbf{k},f}}{\epsilon_{\mathbf{k},c} + \epsilon_{\mathbf{k},f}} \right) \right] \end{aligned}$$

For v_θ , one gets,

$$v_\theta = \left[\frac{\Delta_0 (\epsilon_{\mathbf{k},c}^2 + 2\epsilon_{\mathbf{k},c}\epsilon_{\mathbf{k},f})^2}{k \epsilon_{\mathbf{k},c} + \epsilon_{\mathbf{k},f}} \right]_{node} \quad (2.13)$$

Next step is to determine the doping dependence of various quantities which would be determined by the doping dependence of nodal wave vector. By looking at the cubic equation for the spinon node one can see that the leading doping dependence would be given by, $k_{node} \sim x^{1/3}$. This would give $\epsilon_{k_{node},c} \sim x^{2/3}$ and $\epsilon_{k_{node},f} \sim x^{1/3}$. Using this one can determine the leading order doping dependence of the two velocities as $v_F \sim x^{1/3}$ and $v_\phi \sim x^{1/3}$. This way one expects that the slope of the decrement of superfluid density with temperature to be independent of temperature.

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