THERMODYNAMIC PROPERTIES OF SUPERCONDUCTOR WITH THE COEXISTENCE OF SPIN DENSITY WAVE AND CHARGE DENSITY WAVE

A DISSERTATION
BY
KANPHOT THONGCHAM

Presented in Partial Fulfillment of the Requirements for the
Doctor of Philosophy Degree in Physics
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In this research, the effects of the interplay between spin density wave (SDW) and charge density wave (CDW) on the thermodynamic properties; the SDW and CDW energy gap, critical temperature, gap-to-T_c ratio and specific heat were studied. The self consistent gap equations were derived from the mean field Hamiltonian of the coexistence of SDW and CDW by Green's function method. From gap equations, the thermodynamic properties of the coexistence state were calculated within the assumption that the band width is very large compared to gaps and density of state is constant near Fermi surface. We obtained the analytic expression of zero-temperature gaps, critical temperature and gap-to-T_c ratio. We found that at zero temperature the zero-temperature gaps are suppressed by the interplay. The interplay between SDW and CDW states lead to their competition, which depend on the magnitude of the coupling constants. The critical temperature at the onset of the coexistence state is inversely proportional to the different of the coupling constants. The density of state and the band structure of the coexistence states show that there should be two effective gaps around the Fermi surface. The gap-to-T_c ratio at the onset of the coexistence state can be larger than that of the BCS universal value. These agree with some of the experimental data of cuprate and iron based superconductor. At the onset of the coexistence state, the specific heat jump for the coexistence state to normal state deviates from the typical value of the BCS jump. Our calculation shows the same tendency as the experimental data of iron based superconductor $Ba(Fe_{0.925}Co_{0.075})_2As_2$.

Keywords: spin density wave, charge density wave, critical temperature, gap-to-T_c ratio, specific heat, superconductors

สมบัติเชิงอุณหพลศาสตร์ของตัวนำยวดยิ่งที่มีการร่วมกันของคลื่นความหนาแน่นเชิงสปิน และคลื่นความหนาแน่นเชิงประจุ

บทคัดย่อ

ของ

กันต์พจน์ ทองแช่ม

เสนอต่อบัณฑิตวิทยาลัย มหาวิทยาลัยศรีนครินทรวิโรฒ เพื่อเป็นส่วนหนึ่งของการศึกษา

ตามหลักสูตรปริญญาปรัชญาดุษฎีบัณฑิต สาขาฟิสิกส์

พฤศจิกายน 2557

กันต์พจน์ ทองแช่ม.(2557). *สมบัติเชิงอุณหพลศาสตร์ของตัวนำยวดยิ่งที่มีการร่วมกันของคลื่นความหนาแน่นเชิงสปินและคลื่นความหนาแน่นเชิงประจุ*. ปริญญานิพนธ์ ปร.ด. (ฟิสิกส์). กรุงเทพฯ: บัณฑิตวิทยาลัย มหาวิทยาลัยศรีนครินทรวิโรฒ. คณะกรรมการควบคุม: รองศาสตราจารย์ ดร.พงษ์แก้ว อุดมสมุทรหิรัญ

งานวิจัยนี้ศึกษาผลของการกระทบซึ่งกันและกันของคลื่นความหนาแน่นเชิงสปินและประจุต่อสมบัติเชิงอุณหพลศาสตร์ คือ ช่องว่างพลังงาน , อุณหภูมิวิกฤติ, อัตราส่วนของช่องว่างพลังงานที่ศูนย์สัมบูรณ์ต่ออุณหภูมิวิกฤติ และความจุความร้อน การคำนวณเริ่มจากการหาสมการช่องว่างพลังงานจากแฮมิลโทเนียนสนามเฉลี่ยโดยวิธีการฟังก์ชันของกรีน สมบัติเชิงอุณหพลศาสตร์จึงถูกคำนวณจากสมการช่องว่างพลังงานโดยมีการสมมติว่าความกว้างของแถบพลังงานมีค่ามากกว่าช่องว่างพลังงานมากๆและความหนาแน่นสถานะที่ปริเวณผิวเฟอร์มีมีค่าคงที่ ผลการคำนวณได้สมการเชิงวิเคราห์สำหรับช่องว่างพลังงาน, อุณหภูมิวิกฤติ, อัตราส่วนของช่องว่างพลังงานที่ศูนย์สัมบูรณ์ต่ออุณหภูมิวิกฤติ พบว่าช่องว่างพลังงานมีค่าลดลงเนื่องจากการกระทบซึ่งกันและกันของคลื่นความหนาแน่นเชิงสปินและประจุ การมีผลกระทบซึ่งกันและกันนำไปสู่การแข่งขันกันระหว่างคลื่นความหนาแน่นเชิงสปินและประจุ อุณหภูมิการเปลี่ยนเฟสนั้นลดลงเมื่อผลต่างของความแรงของอันตรกริยามีค่าเพิ่มขึ้น ความหนาแน่นสถานะและแถบพลังงานแสดงให้เห็นว่ามีสองช่องว่างพลังงานยังผล อัตราส่วนของช่องว่างพลังงานที่ศูนย์สัมบูรณ์ต่ออุณหภูมิวิกฤติ ณ อุณหภูมิการเปลี่ยนเฟสมีค่ามากกว่าค่าจากทฤษฎีบีซีเอส ซึ่งสอดคล้องกับผลการทดลองในบางตัวอย่างของตัวนำยวดยิ่งคิวเพรท และตัวนำยวดยิ่งชนิดมีเหล็กเป็นองค์ประกอบหลัก การกระโดดของความจะความร้อนที่สอดคล้องกับการทดลองเป็นการกระโดดของความจุความร้อนจากสถานะที่อยู่ร่วมกันของคลื่นความหนาแน่นเชิงสปินและประจุมายังสถานะปรกติ ซึ่งมีค่าต่างไปจากทฤษฎีบีซีเอส ค่าที่คำนวณได้แสดงแนวโน้มเช่นเดียวกับค่าจากการทดลองของตัวนำยวดยิ่ง $Ba(Fe_{0.925}Co_{0.075})_2As_2$

คำสำคัญ: คลื่นความหนาแน่นเชิงสปิน, คลื่นความหนาแน่นเชิงประจุ, อุณหภูมิวิกฤติ, อัตราส่วนของช่องว่างพลังงานที่ศูนย์สัมบูรณ์ต่ออุณหภูมิวิกฤติ, ความร้อนจำเพาะ, ตัวนำยวดยิ่ง

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by

Kanphot Thongcham

has been approved by the Graduate School as partial fulfillment of the requirements for the Doctor of Philosophy Degree in Physics of Srinakharinwirot University.

…………………………………………… Dean of Graduate School

(Assoc. Prof. Dr. Somchai Santiwatanakul)

November /……./ 2014

Dissertation Committee	Oral Defense Committee
.... Major-advisor (Assoc.Prof.Dr. Pongkaew Udomsamuthirun)	.... Chair (Assoc. Prof. Dr. Udomsilp Pinsook)
	....Committee (Assoc.Prof.Dr. Pongkaew Udomsamuthirun)
	....Committee (Dr. Supitch Khemmani)

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Kanphot Thongcham

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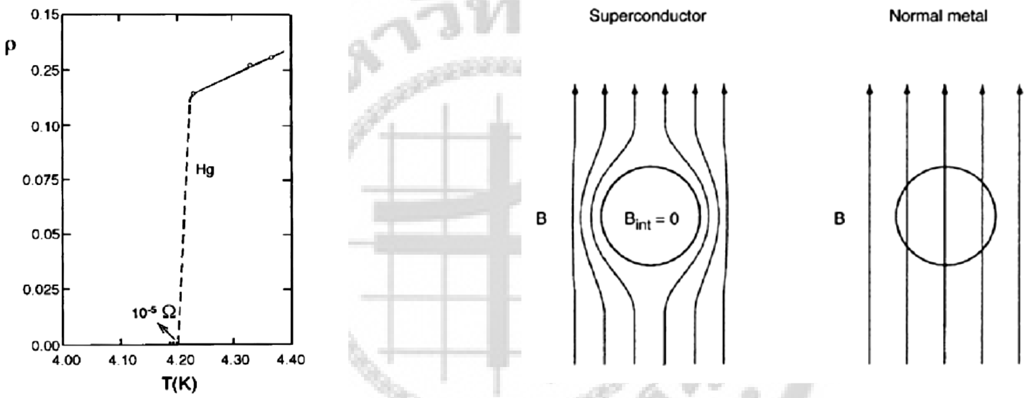
CHAPTER 1
INTRODUCTION

1 Historical Background

In 1911, the phenomenon called “Superconductivity” was first discovered by Heike Kamerlingh Onnes. In the study of electrical resistivity of mercury Hg at low temperature, he found that the resistance of Hg drops suddenly to zero at 4.19 K (figure.1 (a)) and called this new state of Hg as superconducting state (Bennemann; & Ketterson. 2008: 3). After the Onnes’ discovery the superconductivity (SC) was observed in many elements and compounds. The temperature at which material passes into superconducting state or become superconductor is called critical temperature T_c.



(a) (b)

Figure 1 (a) Kamerlingh Onnes’ discovery of vanishing of the electrical resistivity of Hg.: Bennemann; & Ketterson.(2008: 3). (b) Meissner effect.: Bennemann;& Ketterson.(2008: 5).

The superconductors are characterized not only by the disappearance of electrical resistance. They also exhibit the perfect diamagnetic characteristic. In 1933 Meissner and Ochsenfeld have reported that below the critical temperature a magnetic field is expelled from the superconductor (figure 1 (b)), this effect is called Meissner-Ochsenfeld effect. In 1935, London brothers have pointed out that the superconductivity is a quantum phenomenon and they use electrodynamics with two-fluid model to explain the magnetic properties of superconductor. The macroscopic theory of superconductor was proposed by Ginzburg and Landau in 1950. In 1950’s, it had discovered that T_c depends on the mass of material (isotope effect). This discovery leaded Frolich to conclude that lattice vibration or phonon has the contribution to the superconductivity and he had shown that two electrons in a metal can attract each other by interchanging the phonon (Bennemann; & Ketterson. 2008: 5, Buckel. 1991: 29).

In 1957, Bardeen, Cooper and Schrieffer (1957: 1175-1204) proposed the theory of superconductivity called BCS theory. This theory was successful to describe all superconductors known at that time. The basic idea of The BCS theory is that two electrons with opposite spin and momentum can form the so-called Cooper pair via the electron-phonon-electron interaction. In this interaction electrons near the Fermi surface can overcome the Coulomb repulsive force by exchange a virtual phonon leading to attractive interaction. The superconducting state can be described by the wave function of Cooper pair. According to BCS theory, the Cooper pair is in the spin singlet state which is antisymmetric. Thus the spatial part must be symmetric, if the radial part is even the angular part must be symmetric i.e. s, d,… states. In the case of Cooper pair the relative angular momentum is zero corresponding to s state or s-wave. The superconductors described by BCS theory or s-wave superconductors are called Conventional superconductor.

In 1962, Josephson had predicted that the Cooper pair can tunnel through superconducting junction. This prediction called Josephson effect was later confirmed by the experiment and there are many areas of applications (Bennemann; & Ketterson. 2008: 20, Plakida. 2010: 485).

2 High Temperature Superconductor (HTS)

In 1979, it was found that $CeCu_2Si_2$ become superconducting at about 0.5 K (Steglich; et al. 1979: 1892-1896). Due to its large effective mass $CeCu_2Si_2$ is called heavy-electron or heavy-fermion superconductor. Recently, many heavy-fermion superconductors have been discovered; UPt_3, Ube_{13}, UPd_2Al_3 and UGe_2 (Bennemann; & Ketterson. 2008: 1031-1154).

In 1980, superconductivity was found in an organic compound $(TMTSF)_2PF_6$(Jerome; et al. 1980: L95-L98). Later, one found additional other organic superconductors. They show unusual properties such as magnetism and unconventional superconductivity (Wosnitza. 2001: 131–141, Bennemann; & Ketterson, 2008: 1155-1224).

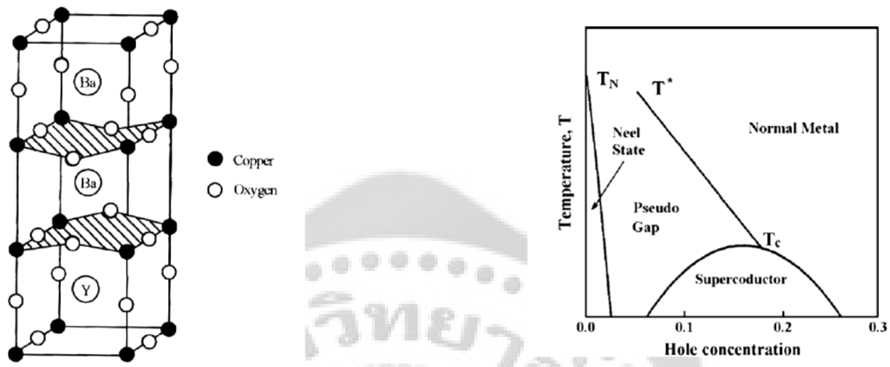
Prior to 1986, most experimentalists and theorists were convinced that the upper limit for the T_c of any superconducting material would be around 23 K for A-15 compound Nb_3Ge (discovered in 1973, Bennemann; & Ketterson. 2008: 4-7). The breakthrough in superconductivity is the discovery by George Bednorz and Alex Muller in 1986 (Bednorz; & Muller. 1986: 189-193). They discovered the superconductivity in $La_{2-x}Ba_xCuO_4$ (LBCO) with T_c about 35 K. This discovery is the beginning of the age of high temperature superconductor (HTS). In 1987, Paul Chu and his colleagues (Wu; et al. 1987: 908-910) found a new material $YBa_2Cu_3O_{6+y}$(YBCO or Y123) with T_c of 92 K. This temperature is above 77 K, the boiling of liquid nitrogen. High-T_c or HTS are material that has T_c above 23.2 K, the upper limit allowed by BCS theory (McMillan limit is about 30 K, McMillan,.1968: 331-344). The superconductors having copper oxide layered structure are called "Cuprates". The classes of cuprate superconductors are shown in Table 1. Now a day, the highest T_c of 138 K is $Hg_{0.8}Tl_{0.2}Ba_2Ca_2Cu_3O_{8.33}$ at ambient pressure and 164 K in $HgBa_2Ca_2Cu_3O_{8+x}$(HBCCO) under high pressure (Gao. 1994: 4260).

All cuprates have the following common feature. The CuO_2 plane; it is believed that the high value of superconducting critical temperature is related to electronic and magnetic structure of the CuO_2 plane (figure2 (a)). Therefore, in theoretical study the cuprates can be considered as two-dimensional material. In CuO_2 plane oxygen (O^{2-}) has a valence configuration of $(1s)^2$ $(2s)^2$ $(2p)^6$ while copper (Cu^{2+}) has configuration $(3d)^9$. For this system the total spin S = 1/2 and the electron at the Cu site is magnetic. Many experiment results after the discovery of cuprate showed that the parent compound of cuprate is anti-ferromagnetic insulator with high Neel temperature, T_N. They become the superconductor under the optimal (hole) doping.

Table 1 Representative classes of cuprate superconductors (Plakida. 2010: 7)

Superconducting compounds	T_c (K)
LMCO-*type compounds*	
$La_{2-x}M_xCuO_4$ (LMCO) M = Ba, Sr, Ca	39
La_2CuO_{4+y}	45
$Ca_{2-x}Na_xCuO_2Cl_2$	26
$R_{2-x}M_xCuO_4$ (RMCO) (electronically doped cuprates)	24
R = Pr, Nd, Sm, Eu, M = Ce, Th, Ce+Sr	
$Sr_{14-x}Ca_xCu_{24}O_{41}$ (ladder compound – superconducting under high pressure at x = 13.6)	12
YBCO-*type compounds*	
RBa2Cu3O6+x (x > 0.4) (R-123) R = Y, La, Ca, RE;	93
RE = Pr, Nd, Sm, Eu, Gd, Dy, Ho, Er, Tm, Yb, Lu	
$YBa_2Cu_4O_8$ (Y-124)	80
$YBa_2Cu_{3.5}O_{8-y}$ (Y-247)	87
$Pb_2Sr_2ACu_3O_{8+y}$, A=R+Sr,R+Ca	80
$La_{2-x}Sr_xCaCu_2O_8$	60
$RuSr_2GdCu_2O_{8-\delta}$ (Ru-1212) (superconducting ferromagnet)	46
Bi-, Tl-, Hg-*type compounds*	
$Bi_2Sr_2Ca_{n-1}Cu_nO_{2n+4+\delta}$ Bi-22(n − 1)n (n = 1–3)	
$Bi_2Sr_2CuO_{6+\delta}$	10
$Bi_2Sr_2Ca_2Cu_3O_{10+\delta}$	110
$Tl_mBa_2Ca_{n-1}Cu_nO_{2n+m+2+\delta}$ Tl-m2(n − 1)n (m = 1, 2; n = 1–4)	
Tl_2Ba_2CuO6+δ 93	
$Tl_1Ba_2Ca_2Cu_3O_{9+\delta}$	133
$Tl_2Ba_2Ca_2Cu_3O_{10+\delta}$	125
$HgBa_2Ca_{n-1}CunO_{2n+2+\delta}$ Hg-12(n − 1)n (n = 1–5)	
$HgBa_2CuO_{4+\delta}$	98
$HgBa_2Ca_2Cu_3O_{8+\delta}$	135
$HgBa_2Ca_2Cu_3O_{8+\delta}$ (under pressure of 30GPa)	164

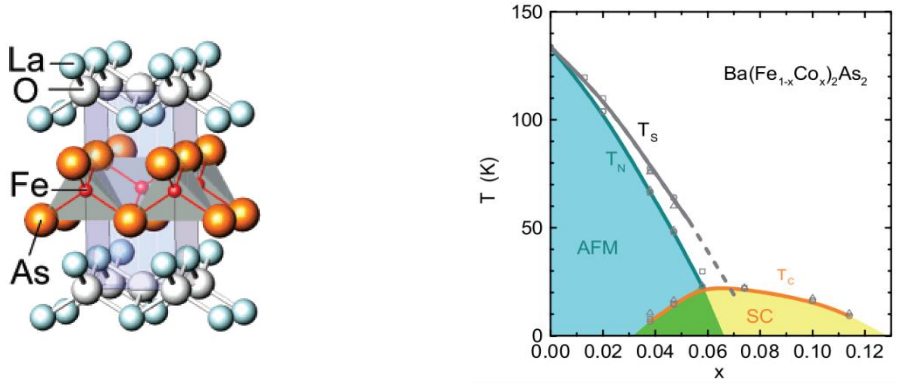
When the charge is removed from CuO_2 planes, their conductivity increase and at optimal doped levels, we can observe a phase transition from the conducting state (normal state) to a superconducting state below T_c. The phase diagram of cuprate is shown in figure.2(b). In the underdoped region, the cuprate exhibit the so-called pseudogap below a characteristic temperature, T^*. In the overdoped region, they are normal metal. From flux quantization measurement reveals that the superconducting state is a result of electron paring or Cooper pairs with charge 2e. The isotope effect of cuprate is very small α = 0.2–0.05, this means that the electron-phonon interaction might has a very small contribution to the mechanism of pairing state. The gap-to-T_c ration of cuprate is rather high(4-8) compared to the BCS value of 3.52, (Gough; et at. 1987: 855, Eremin; & Sunyaev. 2010: 357-359).



(a) (b)

Figure 2 (a) Structure of cuprate $YBa_2Cu_3O_{7-\delta}$.:Bennemann; & Ketterson.(2008: 9) (b) Phase diagram of the cuprate superconductors.:Plakida.(2010: 9)

In 2001, MgB_2 was found to become superconducting below 39 K. It is a s-wave superconductor with two-band crossing the Fermi level (Nagamatsu; et al. 2001: 63-67). In 2008, a new class of superconductors, known as iron-based superconductors, has been discovered in $LaFeAsO_{1-x}F_x$ with T_c of 26 K(Kamihara; et at. 2008: 3296-3297) . Subsequent studies show that replacement of La by other rare earth elements increases T_c, i.e. 41 K for Ce, 52 K for Pr, 52 K for Nd and 55 K for Sm (Ren; et at. 2008: 17002, Chen; et at. 2008: 761-762). Superconductivity is also observed in F-free system $XFeAsO_{1-x}$, X is rare earth elements. Iron-based superconductors containing As are called Fe-Pnictides. Others containing Se or Te are called Fe-Chalcogenides. Similar to high- T_c cuprates, the superconductivity in the iron-based superconductor is related to a layered structure, i.e. FeAs layer. Figure 3(a) demonstrate the phase diagram of LaOFeAs .Generally, it is believed that superconductivity and magnetism are exclusive phenomena. However, the phase diagram of iron based superconductor shows that they can coexist for a specific range of doping as shown in figure 3(b).



(a) (b)

Figure 3 (a)Crystal structure of LaOFeAs.:Kamihara.(2008: 3296-3297). (b) Phase diagram of iron-based superconductor $Ba(Fe_{1-x}Co_x)_2As_2$.: Pratt; et at.(2009: 087001).

If we use the criteria that the HTS is the superconductor with T_c exceed 23 K of Nb_3Ge. There are eight families of HTS, cuprates(1986), $Ba_{1-x}K_xBiO3$(1988), intercalated C_{60}(1991), borocarbide(1994), β-HfNCl(1998), MgB_2(2001), Ca under high pressure(2006) and iron-based superconductor(2008)(Uchida, 2008:9-14). However, if the criteria are that the HTS is the superconductor with T_c exceed the liquid-nitrogen boiling point 77 K, only cuprates can be called the true high-temperature superconductors. The critical temperature T_c of superconductors as a function of time of the discovery is shown in figure 4. In this figure the superconductors are classified into three types; low temperature superconductor (LTS), high temperature superconductor (HTS) and very high temperature superconductor (VHTS).

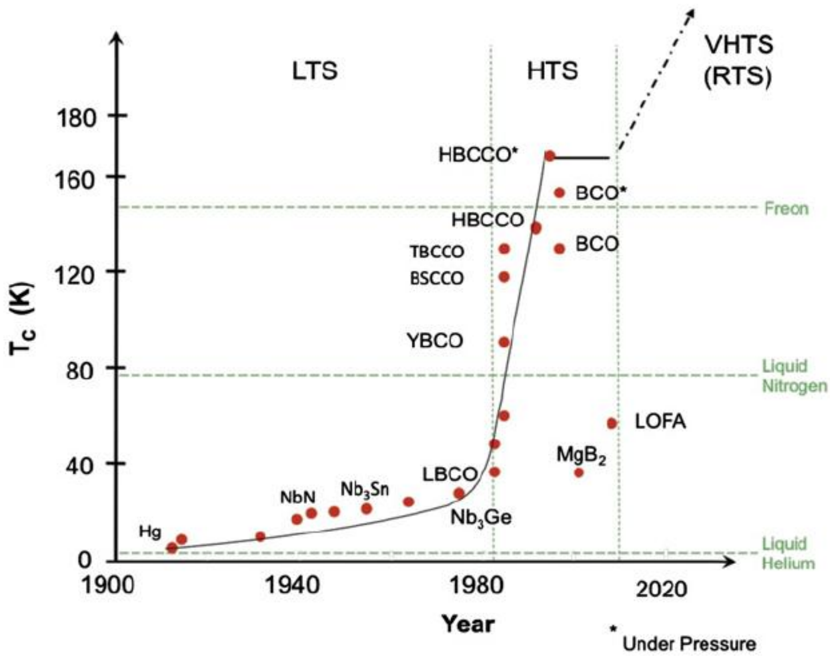


Figure 4 The rising of T_c with time in three different periods: Chu.(2012: 33-44).

Now a day, many researchers are going to understand the mechanism in these High T_c compounds and try to increase the transition temperature T_c. However, the mechanism of paring formation in high T_c is not clearly known. There are many theoretical proposal descriptions for HTS, such as resonant valance bond (RVB) by P.W. Anderson, stripes phase, SO(5) theory(Edegger; et al. 2007: 927-1033), density wave (DW)(Gruner. 1994) and so on.

In this work we focus on the charge density wave and spin density wave (CDW and SDW). SDW and CDW are the broken- symmetry ground states arising from of electron-electron and electron-phonon interaction, respectively. These states have many similarities to the other broken-symmetry ground states of metals, such as superconductivity. The CDW is a static wave of Charge density. The SDW is a static wave of spin density; a kind of antiferromagnetic state with no net magnetization in the entire volume. Thus, the CDW is non magnetic, while the SDW has a magnetic character. Density wave can be observed at low temperature in low dimension materials 1, 2 or quasi-1 dimension. Many experiments show that the density wave can coexist with superconductivity in iron-based and cuprates superconductor (Gabovich; et al. 2002: 583-709). The role of density wave on superconductivity is still under the debate. It is not clear the density wave enhances or suppresses the superconductivity. In additional to the coexistence of density wave with superconductivity the coexistence of the SDW and CDW was also throughout studied. Theoretical interested in the coexistence of the SDW and CDW is stimulated by the observation of SDW/CDW in the superconductor (Pouget; & Ravy. 1997: 1523 -1528, Huxley; et al. 2001: 144519, Fujita; et al. 2004: 104517).

3 The Purpose of the Research

To study the thermodynamic properties ; energy gap, critical temperature and specific heat; of the superconductor having the coexistence of spin density wave and charge density wave.

4 The Importance of the Research

To describe the thermodynamic properties of the superconductor having the coexistence of spin density wave (SDW) and charge density wave (CDW) and to study the interplay between the SDW and CDW.

5 Scope of the Research

To calculate the energy gap, critical temperature and specific heat of the coexistence of the SDW and CDW for two dimension square lattice using the Green's function technique.

CHAPTER 2
THEORETICAL BACKGROUND AND LITERATURE REVIEW

1 BCS Theory

The Froelich Hamiltonian for electron-phonon-electron interaction is

$$H = -\sum_{k,k',q}\sum_{\alpha,\alpha'} V_{k,k+q}\, \hat{c}^{\dagger}_{k+q,\alpha}\hat{c}_{k,\alpha}\hat{c}^{\dagger}_{k'-q,\alpha'}\hat{c}_{k',\alpha'}\,. \tag{2.1}$$

The operator $\hat{c}^{\dagger}_{k,\alpha}(\hat{c}_{k,\alpha})$ creates (annihilates) an electron with wave vector k and spin α. The spin indices $\alpha =\uparrow$ for spin up and $\alpha =\downarrow$ for spin down and $V_{k,k+q}$ is the effective electron-phonon interaction (Froehlich. 1950: 845-856, Mahan. 2000: 628, Fetta; & Walecka. 1971: 439). According to the BCS theory the total momentum and spin of Cooper pair is zero, inserting $k' = -k, \alpha' = -\alpha$ to eq. (2.1) and interchanging the order of operator yields

$$H = -\sum_{k,\alpha,q} V_{k,k+q}\hat{c}^{\dagger}_{k+q,\alpha}\hat{c}^{\dagger}_{-k-q,-\alpha}\hat{c}_{-k,-\alpha}\hat{c}_{k,\alpha}\,. \tag{2.2}$$

Changing the index $k + q \to k'$ and including the electron band energy, we get

$$H = -\sum_{k,\alpha}(\varepsilon_k - \mu)\hat{c}^{\dagger}_{k,\alpha}\hat{c}_{k,\alpha} + \sum_{k,k',\alpha} V_{k,k'}\hat{c}^{\dagger}_{k',\alpha}\hat{c}^{\dagger}_{-k',-\alpha}\hat{c}_{-k,-\alpha}\,\hat{c}_{k,\alpha}. \tag{2.3}$$

Because the interaction is independent of spin index, the last term can be written as

$$\begin{aligned}\sum\nolimits_{k,k'} V_{k,k'}\big(\hat{c}^{\dagger}_{k',\uparrow}\hat{c}^{\dagger}_{-k',\downarrow}\hat{c}_{-k,\downarrow}\hat{c}_{k,\uparrow} + \hat{c}^{\dagger}_{k',\downarrow}\hat{c}^{\dagger}_{-k',\uparrow}\hat{c}_{-k,\uparrow}\hat{c}_{k,\downarrow}\big) = \\ \sum\nolimits_{k,k'} 2V_{k,k'}\hat{c}^{\dagger}_{k',\uparrow}\hat{c}^{\dagger}_{-k',\downarrow}\hat{c}_{-k,\downarrow}\hat{c}_{k,\uparrow}.\end{aligned} \tag{2.4}$$

Including the factor 2 into the interaction strength, we obtain the model Hamiltonian of superconductivity as

$$H_{SC} = \sum_{k,\alpha}(\varepsilon_k - \mu)\hat{c}^{\dagger}_{k,\alpha}\hat{c}_{k,\alpha} - \sum_{k,k'} V_{k,k'}\hat{c}^{\dagger}_{k',\uparrow}\hat{c}^{\dagger}_{-k',\downarrow}\hat{c}_{-k,\downarrow}\hat{c}_{k,\uparrow}. \tag{2.5}$$

The first term is electron band energy measured from the Fermi level μ. The second term represents the effective electron-phonon-electron interaction, $V_{kk'}$ is the strength of the interaction. To solve this Hamiltonian, we apply the mean field technique to H_{SC}. The main idea of mean field technique is to replace a product of two operators with its mean value. This technique is good for the case that the fluctuation is so small. Considering the Hamiltonian $\mathrm{H} = \mathrm{V}\hat{\mathrm{A}}\hat{\mathrm{B}}$, we add and subtract the operator with its mean value. We have

$$\begin{aligned} \mathrm{H} &= \mathrm{V}\hat{\mathrm{A}}\hat{\mathrm{B}} = \mathrm{V}\big(\hat{\mathrm{A}} - \langle\hat{\mathrm{A}}\rangle + \langle\hat{\mathrm{A}}\rangle\big)\big(\hat{\mathrm{B}} - \langle\hat{\mathrm{B}}\rangle + \langle\hat{\mathrm{B}}\rangle\big) \\ &= \mathrm{V}\big(\hat{\mathrm{A}} - \langle\hat{\mathrm{A}}\rangle\big)\big(\hat{\mathrm{B}} - \langle\hat{\mathrm{B}}\rangle\big) + \mathrm{V}\langle\hat{\mathrm{B}}\rangle\hat{\mathrm{A}} + \mathrm{V}\langle\hat{\mathrm{A}}\rangle\hat{\mathrm{B}} - \mathrm{V}\langle\hat{\mathrm{A}}\rangle\langle\hat{\mathrm{B}}\rangle. \end{aligned} \tag{2.6}$$

If the fluctuation is very small, the first term; the 2^{nd} of the fluctuation; can be neglected.

$$\mathrm{H} \approx \mathrm{V}\langle\hat{\mathrm{B}}\rangle\hat{\mathrm{A}} + \mathrm{V}\langle\hat{\mathrm{A}}\rangle\hat{\mathrm{B}} - \mathrm{V}\langle\hat{\mathrm{A}}\rangle\langle\hat{\mathrm{B}}\rangle. \tag{2.7}$$

The average value of the Hamiltonian is

$$\langle\mathrm{H}\rangle = \langle\mathrm{V}\langle\hat{\mathrm{B}}\rangle\hat{\mathrm{A}} + \mathrm{V}\langle\hat{\mathrm{A}}\rangle\hat{\mathrm{B}} - \mathrm{V}\langle\hat{\mathrm{A}}\rangle\langle\hat{\mathrm{B}}\rangle\rangle = \mathrm{V}\langle\hat{\mathrm{A}}\rangle\langle\hat{\mathrm{B}}\rangle. \tag{2.8}$$

Applying eq. (2.8) to the interaction term in eq. (2.5), the Hamiltonian of the superconductor is become

$$\begin{aligned} \mathrm{H_{SC}} = \sum_{\mathrm{k},\alpha}(\varepsilon_{\mathrm{k}} - \mu)\hat{c}^{\dagger}_{\mathrm{k},\alpha}\hat{c}_{\mathrm{k},\alpha} - \sum_{\mathrm{k},\mathrm{k}'}\Big(&\mathrm{V}_{\mathrm{k},\mathrm{k}'}\langle\hat{c}_{-\mathrm{k},\downarrow}\hat{c}_{\mathrm{k},\uparrow}\rangle\hat{c}^{\dagger}_{\mathrm{k}',\uparrow}\hat{c}^{\dagger}_{-\mathrm{k}',\downarrow} \\ &+\mathrm{V}_{\mathrm{k},\mathrm{k}'}\langle\hat{c}^{\dagger}_{\mathrm{k}',\uparrow}\hat{c}^{\dagger}_{-\mathrm{k}',\downarrow}\rangle\hat{c}_{-\mathrm{k},\downarrow}\hat{c}_{\mathrm{k},\uparrow} - \mathrm{V}_{\mathrm{k},\mathrm{k}'}\langle\hat{c}^{\dagger}_{\mathrm{k}',\uparrow}\hat{c}^{\dagger}_{-\mathrm{k}',\downarrow}\rangle\langle\hat{c}_{-\mathrm{k},\downarrow}\hat{c}_{\mathrm{k},\uparrow}\rangle\Big) \end{aligned} \tag{2.9}$$

Dropping the constant term and introducing the order parameter or SC gap

$$\Delta_{\mathrm{k}} = -\sum_{\mathrm{k}'}\mathrm{V}_{\mathrm{k},\mathrm{k}'}\langle\hat{c}_{-\mathrm{k}',\downarrow}\hat{c}_{\mathrm{k}',\uparrow}\rangle = \Delta^{*}_{\mathrm{k}} = -\sum_{\mathrm{k}'}\mathrm{V}_{\mathrm{k},\mathrm{k}'}\langle\hat{c}^{\dagger}_{\mathrm{k}',\uparrow}\hat{c}^{\dagger}_{-\mathrm{k}',\downarrow}\rangle, \tag{2.10}$$

we obtain the mean field Hamiltonian

$$\mathrm{H_{SC}} = \sum_{\mathrm{k},\alpha}(\varepsilon_{\mathrm{k}} - \mu)\hat{c}^{\dagger}_{\mathrm{k},\alpha}\hat{c}_{\mathrm{k},\alpha} + \sum_{\mathrm{k}}\Delta_{\mathrm{k}}\hat{c}^{\dagger}_{\mathrm{k},\uparrow}\hat{c}^{\dagger}_{-\mathrm{k},\downarrow} + \Delta_{\mathrm{k}}\hat{c}_{-\mathrm{k},\downarrow}\hat{c}_{\mathrm{k},\uparrow}. \tag{2.11}$$

For s-wave superconductors, the SC gap is constant for entire Brillouinn zone $\Delta_{\mathrm{k}} = \Delta$ $\big(\mathrm{V}(\mathrm{k},\mathrm{k}') = \mathrm{V}\big)$. Then the model Hamiltonian can be rewritten as

$$\begin{aligned} \mathrm{H} = \sum_{\mathrm{k}}&(\varepsilon_{\mathrm{k}} - \mu)\hat{c}^{\dagger}_{\mathrm{k},\uparrow}\hat{c}_{\mathrm{k},\uparrow} - (\varepsilon_{\mathrm{k}} - \mu)\hat{c}_{-\mathrm{k},\downarrow}\hat{c}^{\dagger}_{-\mathrm{k},\downarrow} \\ &+\Delta\big(\hat{c}^{\dagger}_{\mathrm{k},\uparrow}\hat{c}^{\dagger}_{-\mathrm{k},\downarrow} + \hat{c}_{-\mathrm{k},\downarrow}\hat{c}_{\mathrm{k},\uparrow}\big) + (\varepsilon_{\mathrm{k}} - \mu). \end{aligned} \tag{2.12}$$

To obtain eq.(2.12), we have changed the index $\mathrm{k} \to -\mathrm{k}$ and used the commutation relation $\big[\hat{c}^{\dagger}_{\mathrm{k},\downarrow}, \hat{c}_{\mathrm{k},\downarrow}\big] = 1$. By dropping the constant term, eq.(2.12) can be written in the matrix form or quadratic form as

$$\mathrm{H} = \sum_{k} \begin{pmatrix} \hat{c}_{k,\uparrow}^{\dagger} & \hat{c}_{-k,\downarrow} \end{pmatrix} \begin{pmatrix} \varepsilon_k - \mu & \Delta \\ \Delta & -\varepsilon_k + \mu \end{pmatrix} \begin{pmatrix} \hat{c}_{k,\uparrow} \\ \hat{c}_{-k,\downarrow}^{\dagger} \end{pmatrix} = \sum_{k} \Psi_k^{\dagger} \mathbb{H} \Psi_k \,. \tag{2.13}$$

Where Ψ_k is a 2-component Numbu field operator and

$$\mathbb{H} = \begin{pmatrix} \varepsilon_k - \mu & \Delta \\ \Delta & -\varepsilon_k + \mu \end{pmatrix}. \tag{2.14}$$

The eigenvalues of this Hamiltonian or the energy of the quasi-particles are given by $E^{\pm} = \pm\sqrt{(\varepsilon_k - \mu)^2 + \Delta^2}$. The time domain Green's function of eq.(2.14) is given by

$$\mathbb{G}(k,\tau) = -\langle T_\tau \Psi_k(\tau) \Psi_k^{\dagger}(0) \rangle = -\begin{pmatrix} \langle T_\tau \hat{c}_{k,\uparrow} \hat{c}_{k,\uparrow}^{\dagger} \rangle & \langle T_\tau \hat{c}_{k,\uparrow} \hat{c}_{-k,\downarrow} \rangle \\ \langle T_\tau \hat{c}_{-k,\downarrow}^{\dagger} \hat{c}_{k,\uparrow}^{\dagger} \rangle & \langle T_\tau \hat{c}_{-k,\downarrow}^{\dagger} \hat{c}_{-k,\downarrow} \rangle \end{pmatrix} \tag{2.15}$$

It is clearly seen that the order parameter can be written in term of Green's function as

$$\Delta = -V \sum_{k} \langle \hat{c}_{-k,\downarrow} \hat{c}_{k,\uparrow} \rangle = -V \sum_{k} \mathbb{G}_{12}(k,\tau) \,. \tag{2.16}$$

The time domain Green's function can be expressed in term of the frequency domain Green's function $\mathbb{G}(k, i\omega_n)$ as

$$\mathbb{G}(k,\tau) = T \lim_{\tau \to 0} \sum_{n} e^{-i\omega_n \tau}\, \mathbb{G}(k, i\omega_n). \tag{2.17}$$

Here $\omega_n = (2n+1)\pi T$ is the Matsubara frequency. We use the Matsubara frequency sum rule for reducing Green's function in the simple form.

$$T \sum_{n} g(i\omega_n) e^{-i\omega_n \tau} = \sum_{i} \mathrm{Rez}\left(g(z_j)\right) f(z_j) e^{z_j \tau}. \tag{2.18}$$

Where $f(z_j)$ is Fermi-Dirac distribution function.The frequency domain Greens function can be directly evaluated from $\mathbb{G}(k, i\omega_n) = (i\omega_n - \mathbb{H})^{-1}$,

$$\mathbb{G}(k, i\omega_n) = \frac{1}{(i\omega_n - E^{+})(i\omega_n - E^{-})} \begin{pmatrix} i\omega_n + \varepsilon_k - \mu & \Delta \\ \Delta & i\omega_n - \varepsilon_k + \mu \end{pmatrix}. \tag{2.19}$$

The order parameter or SC gap derived from Green's function takes the form,

$$\Delta = -V \sum_{k} \lim_{\tau \to 0} T \sum_{n} \frac{\Delta e^{-i\omega_n \tau}}{(i\omega_n - E^{+})(i\omega_n - E^{-})} \,.$$

Applying Matsubara sum rule to above equation, we obtain the gap equation

$$\frac{1}{V} = -\sum_k \frac{f(E^+) - f(E^-)}{2E^+} = \sum_k \frac{\mathrm{Tanh}\left(\sqrt{(\varepsilon_k - \mu)^2 + \Delta^2}/2T\right)}{2\sqrt{(\varepsilon_k - \mu)^2 + \Delta^2}}. \tag{2.20}$$

Next we change the summation to the integration over the energy shell $\mu - \omega_D < \varepsilon < \mu + \omega_D$, ω_D denotes the Debye frequency. BCS theory assume that out of this shell the interaction of SC gap is zero. Assuming that in the vicinity of Fermi level the density of states is constant N(0). Thus, the gap equation can be expressed as follow

$$\begin{aligned} \frac{1}{N(0)V} &= \int_0^{\mu+\omega_D} d\varepsilon \frac{\mathrm{Tanh}\left(\sqrt{(\varepsilon - \mu)^2 + \Delta^2}/2T\right)}{\sqrt{(\varepsilon - \mu)^2 + \Delta^2}} \\ &= \int_0^{\omega_D} d\varepsilon \frac{\mathrm{Tanh}\left(\sqrt{\varepsilon^2 + \Delta^2}/2T\right)}{\sqrt{\varepsilon^2 + \Delta^2}}. \end{aligned} \tag{2.21}$$

From eq.(2.21), the behavior of SC gap as a function of temperature can be analyzed. At zero temperature the term Tanh(∞) can be replaced by 1 and after some calculations we arrive at

$$\frac{1}{N(0)V} = \ln\left(\frac{\omega_D + \sqrt{\omega_D^2 + \Delta^2}}{\Delta(0)}\right). \tag{2.22}$$

If the SC gap is so small compared to the Debye frequency, we can approximate the numerator as $\omega_D + \sqrt{\omega_D^2 + \Delta^2} = 2\omega_D$. Then, the at zero-temperature SC gap is

$$\Delta(0) = 2\omega_D e^{-1/\lambda}. \tag{2.23}$$

Here λ=N(0)V denotes the coupling constant.

At the critical temperature T_c the SC gap vanishes, one can finds

$$\frac{1}{\lambda} = \int_0^{\omega_D} d\varepsilon \frac{\mathrm{Tanh}(\varepsilon/2T_c)}{\varepsilon} = \int_0^{\omega_D/2T_c} dx \frac{\mathrm{Tanh}(x)}{x}. \tag{2.24}$$

Applying the by-part integration technique to eq.(2.24), we get

$$\frac{1}{\lambda} = \ln\left(\frac{\omega_D}{2T_c}\right)\mathrm{Tanh}\left(\frac{\omega_D}{2T_c}\right) - \int_0^{\omega_D/2T_c} d\varepsilon \ln(x)\mathrm{Sech}^2(x). \tag{2.25}$$

For simple elemental superconductors, the condition $\omega_D \gg 2T_c$ is hold. Eq.(2.25) can be approximate as following

$$\frac{1}{\lambda} \cong \ln\left(\frac{\omega_D}{2T_c}\right) - \int_0^\infty d\varepsilon \ln(x) \mathrm{Sech}^2(x) = \ln\left(\frac{\omega_D}{2T_c}\right) - \ln\left(\frac{\pi}{4\gamma}\right). \tag{2.26}$$

Where $\gamma \sim 1.78$. Henceforth, the BCS theory predicts that the critical temperature is

$$T_c = \frac{2\omega_D\gamma}{\pi} e^{-1/\lambda}. \tag{2.27}$$

Dividing eq.(2.23) by eq.(2.27), we get the relation between zero-temperature gap and critical temperature

$$\frac{\Delta(0)}{T_c} = \frac{\pi}{\gamma} \approx 1.76. \tag{2.28}$$

This gap-to-T_c ratio is independent from all parameters of the theory, it implies that the ratio $\Delta(0)/T_c$ is a universal constant can be applied to all superconductors.

Next, we consider the SC gap in the vicinity of zero temperature or near zero temperature gap. In the vicinity of zero temperature, the energy of the electron is very small compared to SC gap that we insert the following approximation to eq.(2.21)

$$\mathrm{Tanh}\left(\sqrt{\varepsilon^2 + \Delta^2}/2T\right) \approx 1 - 2e^{-\Delta/T} e^{-\varepsilon^2/2\Delta(0)T}. \tag{2.29}$$

In the vicinity of zero temperature, the gap equation becomes

$$\frac{1}{\lambda} = \int_0^{\omega_D} d\varepsilon \frac{1}{\sqrt{\varepsilon^2 + \Delta^2}} - 2e^{-\Delta(0)/T} \int_0^{\omega_D} d\varepsilon \frac{e^{-\varepsilon^2/2\Delta(0)T}}{\sqrt{\varepsilon^2 + \Delta^2}}. \tag{2.30}$$

In the second term, we change the variable $\varepsilon = x\sqrt{2\Delta(0)T}$ and approximate the denominator as $\sqrt{\varepsilon^2 + \Delta^2} \approx \Delta(0)$. Taking the upper limit to infinity, we have

$$\frac{1}{\lambda} = \ln\left(\frac{2\omega_D}{\Delta(T)}\right) - \sqrt{\frac{2\pi T}{\Delta(0)}} e^{-\Delta(0)/T}. \tag{2.31}$$

Applying eq.(2.23) to the left hand side of eq.(2.31), one find

$$\ln\left(\frac{\Delta(T)}{\Delta(0)}\right) = -\sqrt{\frac{2\pi T}{\Delta(0)}} e^{-\Delta(0)/T}. \tag{2.32}$$

Since the value of $\Delta(T)$ is very closed to $\Delta(0)$,we use the following approximation,

$$\ln\left(\frac{\Delta(T)}{\Delta(0)}\right) = \ln\left(1 + \frac{\Delta(T) - \Delta(0)}{\Delta(0)}\right) \approx \frac{\Delta(T) - \Delta(0)}{\Delta(0)}.$$

Then, we obtain the near zero-temperature gap as

$$\Delta(\mathrm{T}) = \Delta(0) - \sqrt{2\pi\Delta(0)\mathrm{T}}e^{-\frac{\Delta(0)}{\mathrm{T}}}. \tag{2.33}$$

In the vicinity of T_c the SC gap is very small, we applied the following relation to the integrand in eq.(2.21)

$$\frac{\mathrm{Tanh(x)}}{\mathrm{x}} = \sum_{\mathrm{n}=0} \frac{2}{\mathrm{x}^2 + (\pi(\mathrm{n}+1/2))^2}. \tag{2.34}$$

Then, the integrand in eq.(2.12) can be rewritten as

$$\frac{1}{\sqrt{\varepsilon^2+\Delta^2}}\mathrm{Tanh}\left(\frac{1}{2\mathrm{T}}\sqrt{\varepsilon^2+\Delta^2}\right) = 4\mathrm{T}\sum_{\mathrm{n}=0}\frac{1}{\varepsilon^2+\Delta^2+\omega_{\mathrm{n}}^2}.$$

Expanding this series in term of SC gap and keeping only the second order term, we get

$$\frac{1}{\sqrt{\varepsilon^2+\Delta^2}}\mathrm{Tanh}\left(\frac{1}{2\mathrm{T}}\sqrt{\varepsilon^2+\Delta^2}\right) = 4\mathrm{T}\sum_{\mathrm{n}=0}\left(\frac{1}{\varepsilon^2+\Delta^2} - \frac{\Delta^2}{(\varepsilon^2+\omega_{\mathrm{n}}^2)^2}\right).$$

Applying this relation to eq.(2.21), we obtaine

$$\frac{1}{\lambda} = \int_0^{\omega_D} d\varepsilon \frac{\mathrm{Tanh}(\varepsilon/2\mathrm{T})}{\varepsilon} - 4\mathrm{T}\Delta^2\int_0^{\omega_D} d\varepsilon\frac{1}{(\varepsilon^2+\omega_{\mathrm{n}}^2)^2}. \tag{2.35}$$

Applying eq.(2.27) to the left hand side and the integration technique eqs.(2.24-2.26) to the first term on the right hand side of eq.(2.35), we find

$$\ln\left(\frac{2\gamma\omega_D}{\pi\mathrm{T_c}}\right) = \ln\left(\frac{2\gamma\omega_D}{\mathrm{T}}\right) - 4\mathrm{T}\Delta^2\sum_n\int_0^{\omega_D} d\varepsilon\frac{1}{(\varepsilon^2+\omega_{\mathrm{n}}^2)^2}. \tag{2.36}$$

If Debye frequency is very large compared to the critical temperature, the second term on the right hand side can be evaluated as

$$\int_0^{\omega_D} d\varepsilon\frac{1}{(\varepsilon^2+\omega_{\mathrm{n}}^2)^2} = \frac{1}{\omega_{\mathrm{n}}^3}\int_0^{\omega_D/\omega_n}\frac{dx}{(1+x^2)^2} \approx \frac{1}{\omega_{\mathrm{n}}^3}\int_0^{\infty}\frac{dx}{(1+x^2)^2} = \frac{\pi}{4\omega_{\mathrm{n}}^3}.$$

Then, eq.(2.36) takes the form

$$\ln\left(\frac{\mathrm{T}}{\mathrm{T_c}}\right) = -\frac{\Delta^2}{\pi^2\mathrm{T}^2}\sum_{\mathrm{n}}\frac{1}{(2\mathrm{n}+1)^3} \approx -\frac{\Delta^2}{\pi^2\mathrm{T_c}^2}\frac{7}{8}\xi(3). \tag{2.37}$$

Here $\xi(z)$ denotes the Riemann zeta function. Because the temperature is very closed to T_c ,we can approximate the logarithm function as

$$\ln\left(\frac{T}{T_c}\right) = \ln\left(1+\frac{T-T_c}{T_c}\right) \approx \frac{T-T_c}{T_c}.$$

Then, we have the near critical-temperature gap

$$\Delta^2(T) = \frac{8\pi^2}{7\xi(3)} T_c(T_c - T) \rightarrow \Delta(T) = 3.06\sqrt{T_c(T_c - T)}\,. \tag{2.38}$$

By applying eq.(2.28) to eq.(2.38) , we get

$$\Delta(T) = 1.74\Delta(0)\left(1-\frac{T}{T_c}\right)^{1/2}. \tag{2.39}$$

Next, we consider the specific heat at near critical temperature. The entropy of our system can be defined as

$$\begin{aligned} s &= -\sum_{k,i=\pm} f(E^i)\ln[f(E^i)] + \left(1-f(E^i)\right)\ln[1-f(E^i)]\,, \\ &= -2\sum_{k} f(E^+)\ln[f(E^+)] + \left(1-f(E^+)\right)\ln[1-f(E^+)]. \end{aligned} \tag{2.40}$$

The specific heat derived from the entropy is given by

$$c = T\frac{ds}{dT} = \frac{2}{T^2}\sum_{k}\frac{e^{E^+/T}}{\left(e^{E^+/T}+1\right)^2}\left((E^+)^2 - E^+T\frac{dE^+}{dT}\right). \tag{2.41}$$

Changing the summation to the integration and use $E^+ = \sqrt{\varepsilon^2+\Delta^2}$, we get

$$c = \frac{4N(0)}{T^2}\int_0^{\omega_D} d\varepsilon\,\frac{e^{\sqrt{\varepsilon^2+\Delta^2}/T}}{\left(e^{\sqrt{\varepsilon^2+\Delta^2}/T}+1\right)^2}\left(\varepsilon^2+\Delta^2-\frac{T}{2}\frac{d\Delta^2}{dT}\right). \tag{2.42}$$

Substituting eq.(2.38) into above equation, we get the specific heat as

$$c = \frac{4N(0)}{T^2}\int_0^{\omega_D} d\varepsilon\,\frac{e^{\sqrt{\varepsilon^2+\Delta^2}/T}}{\left(e^{\sqrt{\varepsilon^2+\Delta^2}/T}+1\right)^2}\left(\varepsilon^2+\Delta^2+TT_c\frac{4\pi^2}{7\xi(3)}\right). \tag{2.43}$$

At critical temperature, the specific heat for superconducting state is

$$c_s = \frac{4N(0)}{T_c^2}\int_0^{\omega_D} d\varepsilon\,\frac{e^{\varepsilon/T_c}}{(e^{\varepsilon/T_c}+1)^2}\left(\varepsilon^2+T_c^2\frac{4\pi^2}{7\xi(3)}\right). \tag{2.44}$$

For the normal state, inserting $\Delta = 0$ into eq.(2.42), one finds

$$c_n = \frac{4N(0)}{T_c^2}\int_0^{\omega_D} d\varepsilon \frac{\varepsilon^2 e^{\varepsilon/T_c}}{(e^{\varepsilon/T_c}+1)^2}. \tag{2.45}$$

The difference of specific heat between superconducting and normal state is

$$\Delta c = c_s - c_n = \frac{16N(0)\pi^2}{7\xi(3)}\int_0^{\omega_D} d\varepsilon \frac{e^{\varepsilon/T_c}}{(e^{\varepsilon/T_c}+1)^2}. \tag{2.46}$$

By changing the variable $\varepsilon = xT_c$ and take the limit $\omega_D/T_c \to \infty$, we can evaluate eq.(2.45) and (2.46) as

$$c_n = 4N(0)T_c\int_0^{\infty} dx \frac{x^2 e^x}{(e^x+1)^2} = 4N(0)T_c\frac{\pi^2}{6}, \tag{2.47}$$

$$\Delta c = \frac{16N(0)\pi^2 T_c}{7\xi(3)}\int_0^{\infty} dx \frac{e^x}{(e^x+1)^2} = \frac{8N(0)\pi^2 T_c}{7\xi(3)}. \tag{2.48}$$

Dividing eq.(2.48) by eq.(2.47) , we obtain the specific heat jump over c_n as

$$\frac{\Delta c}{c_n} = \frac{12}{7\xi(3)} = 1.43\,. \tag{2.49}$$

The BCS theory predicts that the ratio $\Delta c/c_n$ is a universal constant, it is independent of any parameters of the system. The specific heat jump at T_c due to the second order phase transition of the normal state to superconducting state.

To determine the specific heat at near zero temperature, we begin by considering the thermodynamics potential

$$\Omega = U - \mu N - TS = \langle H \rangle - TS. \tag{2.50}$$

Here the $\langle \ldots \rangle$ denotes the ensemble average. After some arrangement eq.(2.40) can be expressed as

$$s = -\sum_{k,}\left(\frac{E^+}{T}\mathrm{Tanh}\left(\frac{E^+}{2T}\right) - 2\ln\left(2\mathrm{Cosh}\left(\frac{E^+}{2T}\right)\right)\right). \tag{2.51}$$

Next, we consider the averaged Hamiltonian

$$\langle H \rangle = \sum_k (\varepsilon_k - \mu)\left(\langle \hat{c}^\dagger_{k,\uparrow}\hat{c}_{k,\uparrow}\rangle + \langle \hat{c}^\dagger_{-k,\downarrow}\hat{c}_{-k,\downarrow}\rangle\right) - \frac{\Delta^2}{V}. \tag{2.52}$$

To obtain the last term, we apply eq.(2.8) to the second term in eq.(2.5). Consider the average number of particles

$$\langle \hat{c}^{\dagger}_{k,\uparrow}\hat{c}_{k,\uparrow}\rangle + \langle \hat{c}^{\dagger}_{-k,\downarrow}\hat{c}_{-k,\downarrow}\rangle = \mathbb{G}_{11}(k,\tau) - \mathbb{G}_{22}(k,\tau). \tag{2.53}$$

By using Matsubara sum rule, we can show that

$$\begin{aligned}\mathbb{G}_{11} &= \frac{E^+ + \varepsilon_k - \mu}{2E^+} f(E^+) - \frac{E^- + \varepsilon_k - \mu}{2E^+} f(E^-)\,,\\ \mathbb{G}_{22} &= \frac{E^+ - \varepsilon_k + \mu}{2E^+} f(E^+) - \frac{E^- - \varepsilon_k + \mu}{2E^+} f(E^-)\,.\end{aligned} \tag{2.54}$$

Then, the average number of particle is

$$\langle \hat{c}^{\dagger}_{k,\uparrow}\hat{c}_{k,\uparrow}\rangle + \langle \hat{c}^{\dagger}_{-k,\downarrow}\hat{c}_{-k,\downarrow}\rangle = -\frac{\varepsilon_k - \mu}{E^+}\mathrm{Tanh}\left(\frac{E^+}{2T}\right). \tag{2.55}$$

Applying eqs.(2.12.55) to eq.(2.50) yields

$$\begin{aligned}\Omega = &\sum_k \frac{-(\varepsilon_k - \mu)^2}{E^+}\mathrm{Tanh}\left(\frac{E^+}{2T}\right) - \frac{\Delta^2}{V}\\ &+ \sum_k \left(E^+\mathrm{Tanh}\left(\frac{E^+}{2T}\right) - 2T\ln\left(2\mathrm{Cosh}\left(\frac{E^+}{2T}\right)\right)\right).\end{aligned} \tag{2.56}$$

After some rearrangement, we get

$$\Omega = \Delta^2 \sum_k \frac{1}{E^+}\mathrm{Tanh}\left(\frac{E^+}{2T}\right) - \frac{\Delta^2}{V} - 2T\sum_k \ln\left(2\mathrm{Cosh}\left(\frac{E^+}{2T}\right)\right). \tag{2.57}$$

Applying eq.(2.20) to the first term, we have

$$\Omega = \frac{\Delta^2}{V} - 2T\sum_k \ln\left(2\mathrm{Cosh}\left(\frac{E^+}{2T}\right)\right). \tag{2.58}$$

We can show that the gap equation can be obtained by minimizing Ω with respect to Δ. At near zero temperature the term "Cosh()" can be approximated as

$$\ln\left(2\mathrm{Cosh}\left(\frac{E^+}{2T}\right)\right) \approx \frac{E^+}{2T} + e^{-\Delta(0)/T}e^{-\varepsilon^2/2\Delta(0)T}\,.$$

Replacing 1/V for the first term in eq.(2.58) by eq.(2.23) , we get

$$\Omega = \Delta^2 N(0)\ln\left(\frac{2\omega_D}{\Delta(0)}\right) - \sum_k E^+ + 2Te^{-\Delta(0)/T}e^{-\varepsilon^2/2\Delta(0)T}. \tag{2.59}$$

Changing the summation to the integration, one finds

$$\Omega = \Delta^2 \mathrm{N}(0)\ln\left(\frac{2\omega_D}{\Delta(0)}\right) - 2\mathrm{N}(0)\int_0^{\omega_D} d\varepsilon\sqrt{\varepsilon^2+\Delta^2}$$
$$+4\mathrm{TN}(0)\sqrt{2\Delta(0)\mathrm{T}}e^{-\Delta(0)/\mathrm{T}}\int_0^{\omega_D/\sqrt{2\Delta(0)\mathrm{T}}} dx\, e^{-x^2}. \tag{2.60}$$

After integration by taking the upper limit of the last term to infinity, we have

$$\Omega \approx -2\mathrm{N}(0)\left(\omega_D^2 + \frac{\Delta(0)^2}{2} + \Delta(0)^2 \mathrm{Log}\left[\frac{2\omega_D}{\Delta(0)}\right]\right)$$
$$+4\mathrm{TN}(0)\sqrt{2\Delta(0)\pi\mathrm{T}}e^{-\Delta(0)/\mathrm{T}} + \Delta^2\mathrm{N}(0)\ln\left(\frac{2\omega_D}{\Delta(0)}\right). \tag{2.61}$$

The entropy near zero temperature calculated from eq.(2.61)is

$$s = -\frac{\partial\Omega}{\partial \mathrm{T}} \approx 2\mathrm{N}(0)\big(\Delta(0)\big)^{\frac{3}{2}}e^{-\frac{\Delta(0)}{\mathrm{T}}}\sqrt{\frac{2\pi}{\mathrm{T}}}. \tag{2.62}$$

The specific heat calculated from entropy is

$$c = \mathrm{T}\frac{\partial S}{\partial \mathrm{T}} \approx 2\mathrm{N}(0)\sqrt{\frac{2\pi}{\mathrm{T}^3}}\big(\Delta(0)\big)^{\frac{5}{2}}e^{-\frac{\Delta(0)}{\mathrm{T}}}. \tag{2.63}$$

2 Density Wave

Charge Density Wave (CDW) was first introduced by Sir Rudolph Peierls in 1950 (Thorne. 1996: 42-47), he predicted that at zero temperature the one dimension metal is not stable. There will be the coupled modulation of the electron density and the lattice distortion (figure 5). This modulation creates the static wave of charge density with the wavelength $\lambda = \pi/k_F$ and introduces the energy gap at the Fermi level. If the temperature increases the energy gap will be decreased and disappear at the transition temperature T_{CDW}. At this temperature the metal-insulator phase transition called Peierls transition takes place. The CDW exhibits the insulating behavior, while the SC state exhibits zero resistivity.

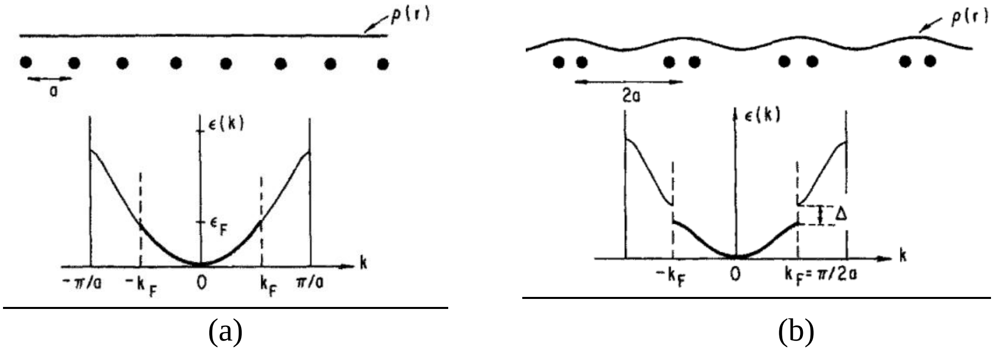


Figure 5 The single particle band, electron density, and lattice distortion in the metallic state above T_{CDW} (a) and in the charge density wave state at T = 0 (b). This figure is appropriate for a half-filled band.:Gruner.(1994:45)

Spin Density Wave (SDW) was proposed by A. W. Overhauser in 1962(Overhauser. 1962: 1437-1452) to describe the paramagnetic state of electron gas. SDW can be viewed as the combination of two CDW with opposite spin and phase different of $\lambda/2$. Like CDW, below the critical temperature SDW introduce the energy gap at the Fermi level.

In order to study the Density Wave (DW), we follow the description by G.Gruner(Gruner. 1994: 1-14).According to Linear response theory, the electron gas will response to the external potential given by

$$\phi(\vec{r}) = \int_q \phi(\vec{q}) e^{i\vec{q}\cdot\vec{r}} d\vec{q}\,, \tag{2.64}$$

by rearranging themselves with the induced charge,

$$\rho^{ind}(\vec{r}) = \int_q \rho^{ind}(\vec{q}) e^{i\vec{q}\cdot\vec{r}} d\vec{q}\,. \tag{2.65}$$

The relation between the induced charge and the potential is

$$\rho^{ind}(\vec{q}) = \chi(\vec{q})\phi(\vec{q})\,. \tag{2.66}$$

Where $\chi(\vec{q})$ is Lindhard response function. In n dimension the response function is

$$\chi(\vec{q}) = \int \frac{d\vec{k}}{(2\pi)^n} \frac{f_k - f_{k+q}}{\varepsilon_k - \varepsilon_{k+q}}\,. \tag{2.67}$$

Here f_k denotes the Fermi-Dirac distribution function. At zero temperature, the response function for the one dimension electron gas is given by

$$\chi(\vec{q}) = N(\varepsilon_F) \ln\left|\frac{q + 2k_F}{q - 2k_F}\right|. \tag{2.68}$$

Here $N(\varepsilon_F)$ is the density of state near Fermi level. It is clearly seen that Eq.(2.68) diverges at $q = 2k_F$. This means that the system of one dimension electron gas is not stable at zero temperature. The stable phase is the periodic pattern of charge density with wave vector $q = 2k_F$ or the wavelength $\lambda = \pi/k_F$. This formation is called "Charge Density Wave". The divergence of the response function $\chi(\vec{q})$ is related to the topology of the Fermi surface. If we consider eq.(2.67) it reveals that the most of the value of the integration comes from the pair of states with equal energy $\varepsilon_k = \varepsilon_{k+q}$, one is below and the other one is above the Fermi level ,and their wave vector is $q = 2k_F$. This means that DW is the result of the paring state of two states near the Fermi surface with $q = 2k_F$. Figure 6 shows the Fermi surface for 1 D electron gas, the Fermi surface are straight line (or point) at k_F and $-k_F$. The Fermi surface is connected by the constant vector $\vec{q}$ called nesting vector. We might summarize that the DW is a result of the nesting of the Fermi surface.

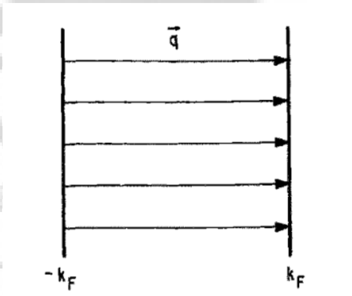


Figure 6 Fermi surface of 1D electron gas.:Gruner.(1994: 45)

In addition to the 1 D material, the DW can also be observed in quasi 1D or 2D materials; the material with chain like structure or the anisotropic material. Consider the example of 2 D material with the tight binding energy

$$\varepsilon(k) = \varepsilon_o + 2t_a\cos(k_x a) + 2t_b\cos(k_y b). \tag{2.69}$$

Here t_a and t_b are hopping integral for x- and y-direction, respectively. For chain like structure; $t_a \gg t_b$;the equation of the Fermi surface derived from eq.(2.6) is

$$k_x = \pm k_F \pm \frac{2t_b}{v_F}\cos(k_y b)\,. \tag{2.70}$$

The Fermi surface corresponds to eq.(2.70) is shown in figure 7. With the nesting vector is $\vec{Q} = (2k_F, \pi/b)$. This nesting vector lead to the divergence of the response function for $\vec{q} = \vec{Q}$. The property of nesting vector is that we can obtain the next Fermi surface by dragging the first sheet of Fermi surface along the nesting vector. If nesting vector is the ratio of reciprocal vector, DW is called commensurate otherwise is incommensurate.

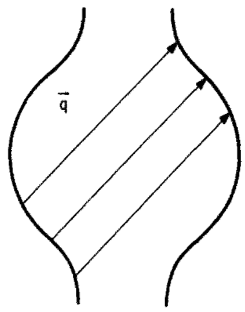


Figure 7 Fermi surface corresponding to eq.(2.2.7).:Gruner.(1994: 45).

Next, we consider eq.(2.67) at any temperature and assuming the density of states near the Fermi surface is constant $N(\varepsilon_F)$. After some calculation, the response function of the state with $q = 2k_F$ takes the form

$$\chi(q = 2k_F, T) = N(\varepsilon_F)\ln\left(\frac{1.143\varepsilon_F}{T}\right). \tag{2.71}$$

In addition to the external potential ϕ^{ext}, there is the induced potential ϕ^{ind} resulting from the induced charge ρ^{ind} . The induced potential is assumed be proportional to the induced charge $\phi^{ind} = U\rho^{ind}$. From eq.(2.66), we obtain the response function as follow

$$\rho^{ind}(\vec{q}) = \chi(\vec{q})\phi(\vec{q}) = \chi(\vec{q})\left(\phi^{ext}(\vec{q}) + \phi^{ind}(\vec{q})\right) = \chi(\vec{q})\left(\phi^{ext}(\vec{q}) + U\rho^{ind}\right).$$

After some rearrangement, we have

$$\rho^{ind}(\vec{q}, T) = \frac{\chi(\vec{q}, T)\phi^{ext}(\vec{q})}{1 - U\chi(\vec{q}, T)}. \tag{2.72}$$

At the critical temperature eq.(2.72) is divergent for $U\chi(\vec{q}, T_c) = 1$. Applying eq.(2.71) to this relation, we obtain the critical temperature

$$T_c = 1.143\varepsilon_F e^{-1/UN(\varepsilon_F)} . \tag{2.73}$$

At this point, we can conclude that DW is the pairing state resulting from the nested Fermi surface. To observe the DW, there are various techniques such as X-ray, neutron or electron diffraction to observe the lattice distortion, scanning tunneling microscopy (STM) to observe the surface of the sample directly, magnetic neutron scattering to observe the magnetic order, resistivity or susceptibility measurement as well as thermal properties measurement; i.e. specific heat.

3 Relevant Research of the Coexistence of the SDW and CDW

Prior to observe the coexistence of SDW and CDW, it has been believed that SDW and CDW cannot coexist. Because their mechanisms are exclusive phenomena, the mechanism induces the SDW is repulsive electron-electron interaction while CDW arises from the attractive electron-phonon interaction. However, many theoretical studies predict the possibility of coexistence of the SDW and CDW. The first study by Denley and Falieov in 1978(1978: 1289-1296), they studied the possible states of 2H-$NbSe_2$ by using the model Hamiltonian

$$H = \sum_{i,j,\sigma} t_{ij} a_i^{\dagger} a_j + U \sum_i n_{i\uparrow} n_{i\downarrow}. \tag{2.74}$$

Here t_{ij} is a hopping integral and U is interaction parameter. In this study, there are many possible stable states depends on the parameter U; (a) the normal paramagnetic state, (b) the ferromagnetic state, (c) a single charge-density wave, (d) a triple charge-density wave, (e) a novel asymmetric charge-density wave, (f) a single spin-density wave, or (g) a mixed state.Their real space pictures are shown in figure 8.

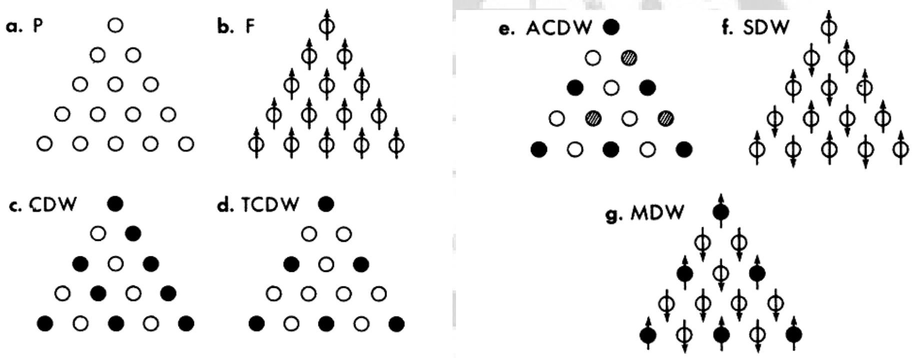
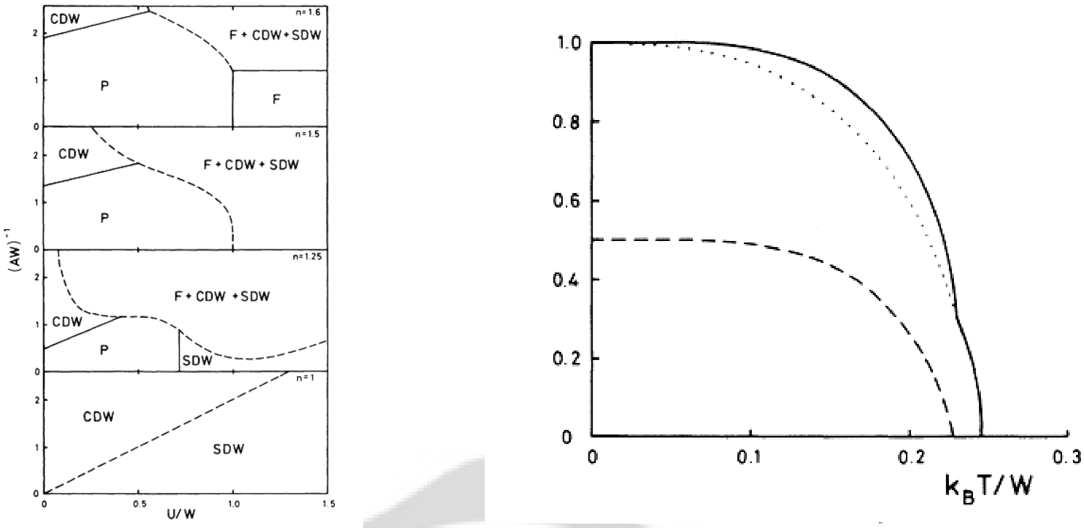


Figure 8 The seven stable states arising from model Hamiltonian eq.(2.74).:Denley;& Falieov.(1978: 1289-1296)

In 1980, Balseiro, Schlottmann and Yndurain (1980: 5267-5271) analyzed the following model Hamiltonian

$$H = \sum_{k,\alpha} \varepsilon_k \hat{c}_{k,\alpha}^{\dagger} \hat{c}_{k,\alpha} + \sum_{k,k',q} U \hat{c}_{k+q,\uparrow}^{\dagger} \hat{c}_{k,\uparrow} \hat{c}_{k'-q,\downarrow}^{\dagger} \hat{c}_{k',\downarrow} - \sum_{k,\alpha} \tau_k \hat{c}_{k+Q,\alpha}^{\dagger} \hat{c}_{k,\alpha} + A\tau^2. \tag{2.75}$$

The first term represents the electron band energy, U is the Coulomb repulsion between electrons at the same site, τ_k a matrix element proportional to the lattice distortion and A is elastic constant. Some of their results are shown in figure 9, F and P denote the ferromagnetic and paramagnetic state, respectively.



(a) (b)

Figure 9 (a) the phase diagram for different occupation number n , W denotes electronic band width, (b) m (magnetization) (full line) and τ/W(CDW) (dashed line) as a function of the temperature for U/W =1.2, (A /W) =2, and n =1.5. The dotted line represents the magnetization for τ =0.: Balseiro; Schlottmann;& Yndurain (1980: 5267-5271)

In1982, Kivelson and Heim (1982: 4278-4292) considered the competing effects of the electron-electron Hubbard repulsion(U) and the electron-phonon Peierls nteraction (α) on the properties of a one-dimensional electron gas. The SCW and CDW can coexist under the appropriate value of parameters, region II in figure 10.

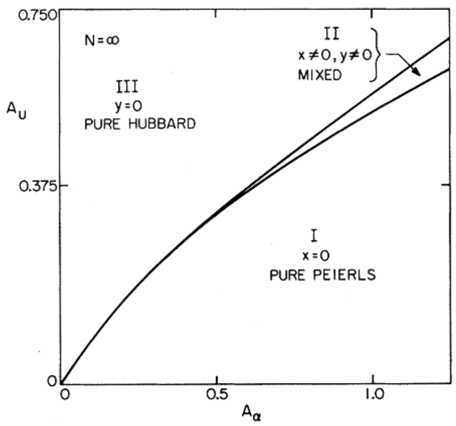


Figure 10 phase diagram of one-dimensional electron gas described by Su-Schrieffer-Heeger model.: Kivelson; & Heim.(1982: 4278-4292)

In 1986, Butz et al (1986: 639-642) reported the first evidence for the coexistence of the SDW and CDW in a two-dimensional material. They studied SDW and CDW in 2H-TaS_2 by using the method of time-differential perturbed angular correlation on ^{181}Ta.

In 1997, Pouget and Ravy(1997: 1523-1528 used X-ray scattering study organic superconductor $(TMTSF)_2PF_6$ and $(TMTTF)_2Br$. They observed the coexistence of $2k_F$ SDW and $2k_F$ CDW. This work stimulates all of the subsequent study of the coexistence of SDW and CDW in organic material (Tomio and Suzumura, 2001: 431-434, Wei et al.,2001: 305–309 , Zhao,Gong and Wang, 2007: 44–48, Katono et al.2012: 1827–1830). By taking into account repulsive interactions of both on-site and nearest-neighbor sites, it has been demonstrated that $2k_F$-SDW can coexists with $4k_F$-CDW.

In 2000, Lin et al (2000:1-23) analyzed the one dimension extended Hubbard model

$$H = -t\sum_{i,\sigma}\left(a_{i\sigma}^{\dagger}a_{i+1\sigma} + \mathrm{h.c.}\right) + U\sum_{i} n_{i\uparrow}n_{i\downarrow} + V\sum_{i} n_i n_{i+1}. \tag{2.76}$$

Where U representing the repulsion when two electrons occupy the same site and V a nearest-neighbor Coulomb repulsion. The phase diagram for band filling =1 is shown in figure 11.

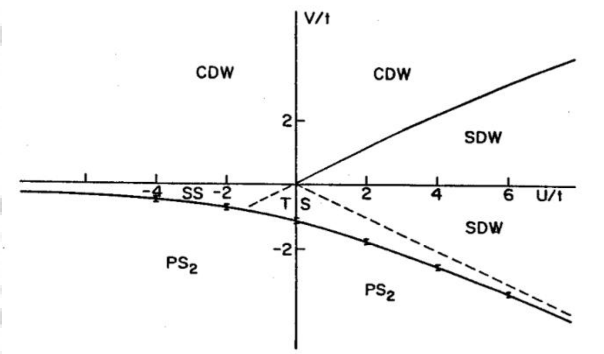


Figure 11 The phase diagram of one-dimensional extended Hubbard model at band-filling = 1. The dashed lines are U = -2V and U = 2V, respectively. : Lin; et al.(2000: 1-23).

There are various types of stable states in a phase diagram. PS_1 and PS_2 are phase separation. In a static PS_1 state, the electrons form a cluster of singly occupied sites while in a static PS_2 state, the electrons form a cluster of doubly occupied sites.

In 2001, Huxley et al(2001: 144519) had shown that superconductivity in UGe_2 has only been detected in the ferromagnetic phase. Additional to the change of slope at the Curie temperature, they observed a second sharp change in the slope of the resistivity at a low temperature, T_x(P). They believed that T_x might correspond to a second phase transition facilitated by a special geometry of the Fermi surfaces. This might lead to the formation of SDW/CDW. Watanbe and Miyake (2002: 115-117, 2002:1465-68) analyzed the specific heat of UGe_2 measured by Huxley. They proposed that the fluctuations related to T_x play an essential role in the mechanism of superconductivity. T_x is considered as the onset temperature of coupled CDW- SDW ordering. The Debye or acoustic mode contribution to specific heat is given as

$$\frac{C_D}{T} = \frac{9Nk_B}{2\omega_D^3}\left[\frac{4}{T^2}\int_0^{\omega_D} d\omega \frac{\omega^3}{e^{\omega/T}-1} - \frac{\omega_D^4}{T^2}\frac{1}{e^{\omega/T}-1}\right].$$

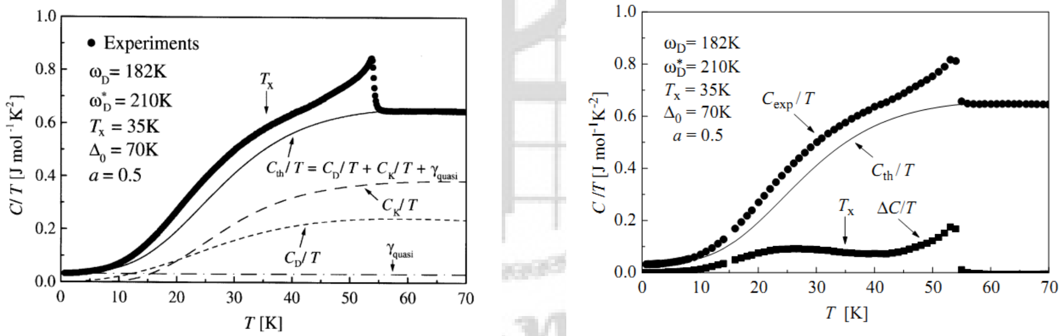
The contribution from optical phonon or Kohn anomaly is

$$\frac{C_D}{T} = \frac{12Nk_B}{\omega_D^{*3}}\left[\frac{1}{T^3}\int_0^{\omega_D^*} d\omega_z \int_0^{\omega_D^*} d\omega\omega \frac{\varepsilon^3 e^{\varepsilon/T}}{(e^{\varepsilon/T}-1)^2} - \frac{1}{2T}\frac{\partial\Delta^2}{\partial T}\int_0^{\omega_D^*} d\omega_z \int_0^{\omega_D^*} d\omega \frac{\omega}{\varepsilon}\frac{(\varepsilon/T-1)e^{\varepsilon/T}+1}{(e^{\varepsilon/T}-1)^2}\right].$$

To calculate the specific heat of UGe_2, they introduce a parameterization for T - dependence of Δ as follows

$$\Delta = \frac{\Delta_0^2\left(T^2 - T_x^2\right)^2}{T_x^4 + aT^4}.$$

The comparison of the experimental data and the theoretical model is shown in figure 12 , γ_{quasi} denotes the Sommerfeld constant.

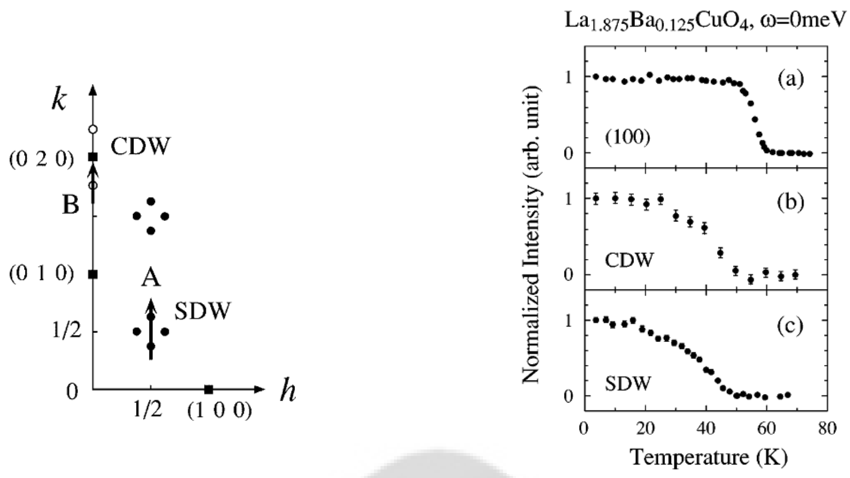


(a) (b)

Figure 12 (a) C/T vs. T : Watanbe;& Miyake.(2002: 115-117) (b)Difference of C= T between experiment and model.:Watanbe and Miyake.(2002:1465-68)

The origin of ΔC/T near $T = T_c$ is the magnetic entropy of the local component of the magnetization, while that of a hump around T = 30K may be attributed to the mass enhancement of quasiparticles due to the criticality of coupled CDW–SDW ordering at $T = T_x$= 35K.

In 2004, Fujita et al (2004: 104517) used a neutron scattering to study a single crystal of $La_{1.875}Ba_{0.125}CuO_4$. Figure 13 shows the results of neutron scattering measurement that have Bragg peak and superlattice peak of SDW and CDW as well as their temperature dependence. In this work, they can conclude that SDW and CDW transition are observed at about 50 K.



(a) (b)

Figure 13 (a) Scan geometry in the (hk0) tetragonal plane. Solid squares show nuclear Bragg peaks; open and solid circles denote nuclear and magnetic IC superlattice peaks, respectively,(b)Temperature dependences of (a)(100), (b) CDW, and (c) SDW superlattice peak intensities in $La_{1.875}Ba_{0.125}CuO_4$.: Fujita et al.(2004: 104517)

In 2008, Fujita et al (2008: 3167-3170) observed SDW and CDW in $La_{1.87}Sr_{0.13}Cu_{0.99}Fe_{0.01}O_4$. The CDW is first observed at about 60 K and SDW subsequently appears at a lower temperature of about 50 K (figure 14).

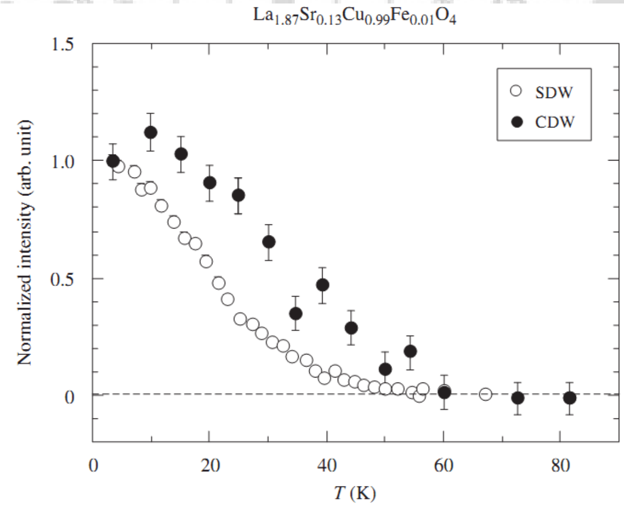


Figure 14 Temperature dependencies of SDW (open circles) and CDW (closed circles) superlattice peak intensities for $La_{1.87}Sr_{0.13}Cu_{0.99}Fe_{0.01}O_4$.: Fujita et al.(2008: 3167-3170).

They also observed SDW and CDW in $La_{1.875}Ba_{0.125}Cu_{0.97}Zn_{0.03}O_4$ by elastic neutron scattering measurements (Fujita; et al. 2008: 1044-1046, Fujita; et al. 2009: 243–245, Fujita. 2012: 23–30). Figure 15 shows the temperature dependence of SDW and CDW, they simultaneously disappear at 30 K.

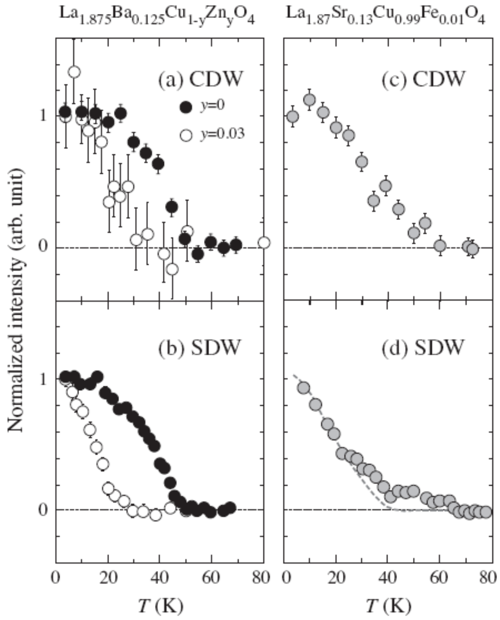


Figure 15 Temperature dependence of the normalized peak-intensity associated with the appearance of (a,c) CDW and (b,d) SDW orders.:Fujita.(2012: 23-30).

In 2008, Pradhan et al (2008: 2332-2335) studied the interplay of SDW and CDW in high T_c superconductors by using the model Hamiltonian

$$H = \sum_{k,\alpha} (\varepsilon_k - \mu) c_{k\alpha}^{\dagger} c_{k\alpha} + \Delta_c \sum_{k,\alpha} c_{k\alpha}^{\dagger} c_{k+Q\alpha} + \Delta_s \sum_{k,\alpha} \sigma c_{k\alpha}^{\dagger} c_{k+Q\alpha}. \tag{2.77}$$

Where the CDW and SDW gap are defined as

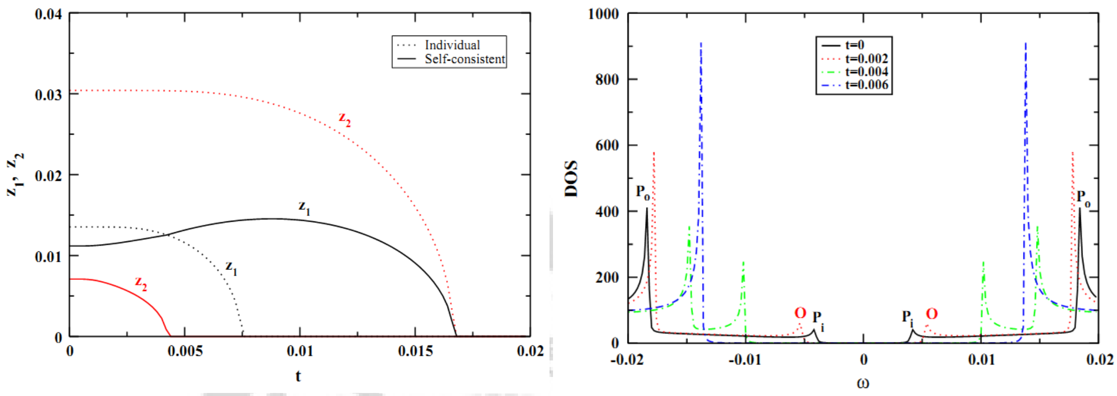
$$\Delta_c = V_1^o \sum_{k,\alpha} \langle c_{k\alpha}^{\dagger} c_{k+Q\alpha} \rangle, \qquad \Delta_s = V_2^o \sum_{k,\alpha} \sigma \langle c_{k\alpha}^{\dagger} c_{k+Q\alpha} \rangle. \tag{2.78}$$

After applying the Zubarev’s technique of double time Green’s function to the model Hamiltonian they obtain the gap equations

$$\Delta_s = \frac{g_2}{2} \int_{-W/2}^{W/2} d\varepsilon_k \left(\frac{(\Delta_c + \Delta_s)}{\omega_1} \mathrm{Tanh}\left(\frac{\omega_1}{2T}\right) - \frac{(\Delta_c - \Delta_s)}{\omega_2} \mathrm{Tanh}\left(\frac{\omega_2}{2T}\right) \right), \tag{2.79}$$

$$\Delta_c = \frac{g_1}{2} \int_{-W/2}^{W/2} d\varepsilon_k \left(\frac{(\Delta_c + \Delta_s)}{\omega_1} \mathrm{Tanh}\left(\frac{\omega_1}{2T}\right) + \frac{(\Delta_c - \Delta_s)}{\omega_2} \mathrm{Tanh}\left(\frac{\omega_2}{2T}\right) \right). \tag{2.80}$$

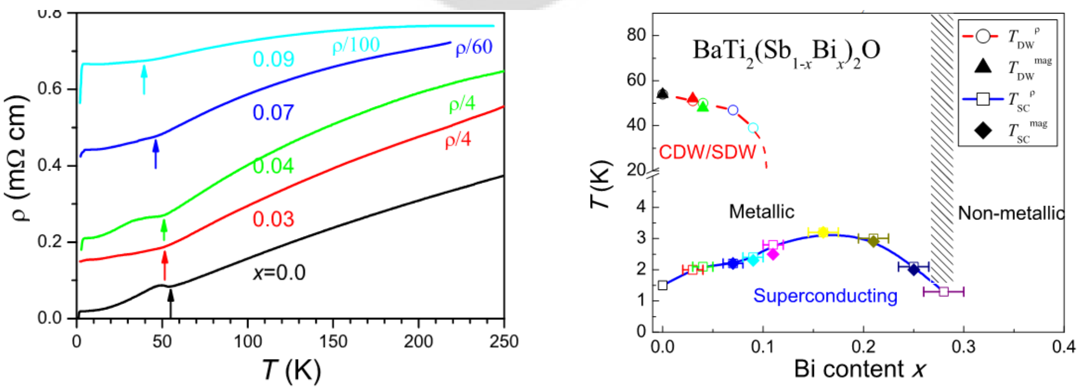
Where the coupling constant $g_c = V_1^o N(0)$, $g_s = V_2^o N(0)$ and the quasi-particle band $\omega_{1,2} = \sqrt{\varepsilon_k^2 + (\Delta_c \pm \Delta_s)^2}$. The self-consistent solutions of these two equations were studied numerically. The interplay between CDW gap z_1 and SDW gap z_2 for g_1 = 0.026 and g_2 = 0.035 is shown in figure 16(a). The DOS at various temperatures are shown in figure 16(b). Fig.16 shows that the gaps are suppressed compared to the individual gaps and the interplay suppresses SDW critical temperature while the CDW critical temperature is enhanced. The gap-to-T_c ratio $2\Delta_c/T_{cdw}$ = 1.31 is smaller than the BCS value of 3.54.



(a) (b)

Figure 16 (a) Temperature dependence of CDW and SDW gaps for the CDW coupling constant g_1 = 0.026 and SDW coupling constant g_2 = 0.035 , dotted lines is individual gap.(b) Density of states plots for different temperatures t =0, 0.002, 0.004 and 0.006.: Pradhan; et al.(2008: 2332-2335).

In 2013, Zhai et al (2013: 100502(R)) showed that SDW and CDW can be seen in $BaTi_2(Sb_{1-x}Bi_x)_2O$. $BaTi_2Sb_2O$ exhibited superconductivity at 1.5 K and CDW/SDW below 54 K. The Bi doping enhances the SC critical temperature to maximum T_c = 3.2 K at x = 0.16. In $BaTi_2(Sb_{1-x}Bi_x)_2O$, Ti_2O sheets can be viewed as CuO_2- planes of cuprate. In this work the DW state is interpreted in term of the structural distortion which is indicated by the increase of the c/a ratio. The temperature dependence of resistivity and phase diagram of $BaTi_2(Sb_{1-x}Bi_x)_2O$ is shown in figure17.



(a) (b)

Figure 17 (a)Temperature dependence of resistivity of the $BaTi_2(Sb_{1-x}Bi_x)_2O$. The arrows mark the CDW/SDW transitions.(b) phase diagram of $BaTi_2(Sb_{1-x}Bi_x)_2O$.: Zai; et al.(2013: 100502(R))

CHAPTER 3
RESEARCH METHODOLOGY

As point out before that the role of density wave on the superconductivity is not clearly known. It is not clear that the density wave enhances or complete with the superconductivity. In this chapter the thermodynamic properties of the coexistence of the SDW and CDW will be derived. Our result can be applied to the superconductivity because the density wave is mathematically generalization of superconductivity. In order to study the coexistence of SDW and CDW in this chapter we will derive the useful formulas which are related to their thermodynamics properties. Firstly, we apply the mean field approximation to the model Hamiltonian of the coexistence of SDW and CDW. Then the gap equations are derived from the mean field Hamiltonian using the Green's function technique. From the Green's function and gap equation several properties such as density of state, free energy, critical temperature and specific heat will be derived under some approximation assumptions.

1 Model Hamiltonian of the Coexistence of the SDW and CDW

Following Balseiro and Falicov(Balseiro; & Falicov. 1979: 4457-4464) ,Schrieffer et al (Schrieffer; et al. 1989: 11664-11679) and Behera(Behera; & Bhattacharya.1990: 112-126) the effective Hamiltonian of the density wave (DW) read as

$$H_{DW} = -\sum_{k,k',q}\sum_{\substack{\alpha,\alpha' \\ ,\beta,\beta'}} V^{DW}_{\alpha\alpha'\beta\beta'}(k,k',q)\hat{c}^{\dagger}_{k+q,\alpha'}\hat{c}_{k,\alpha}\hat{c}^{\dagger}_{k'+q,\beta'}\hat{c}_{k',\beta}\,. \tag{3.1}$$

This can be seen that the DW state can be consider as the generalization of the superconductivity state. For s-wave superconductor electrons with the opposite momentum and spin pair. In the DW state the pairing occur between the states with momentum differing by a fixed momentum Q. For SDW Hamiltonian putting

$$V^{DW}_{\alpha\alpha'\beta\beta'}(k,k',q) = \frac{V^s}{2}\delta(q-Q)\sigma^z_{\alpha'\alpha}\sigma^z_{\beta'\beta} \tag{3.2}$$

this means that the most contribution to the Hamiltonian come from the wave vector q = Q, the nesting vector. Then the SDW Hamiltonian is

$$H_{SDW} = -\sum_{k,k'}\sum_{\substack{\alpha,\alpha' \\ ,\beta,\beta'}} \frac{V^s}{2}\hat{c}^{\dagger}_{k+Q,\alpha'}\sigma^z_{\alpha'\alpha}\hat{c}_{k,\alpha}\hat{c}^{\dagger}_{k'+Q,\beta'}\sigma^z_{\beta'\beta}\hat{c}_{k',\beta}.$$

To simplify this Hamiltonian we apply the mean field technique to H_{SDW}. The main idea of mean field technique is to replace a product of two operators by its mean value. This technique is good if the fluctuation is negligibly small. The mean field Hamiltonian can be derived as following, replacing

$\hat{c}^{\dagger}_{k+Q,\alpha'}\sigma^{z}_{\alpha'\alpha}\hat{c}_{k,\alpha}$ by $\left(\hat{c}^{\dagger}_{k+Q,\alpha'}\sigma^{z}_{\alpha'\alpha}\hat{c}_{k,\alpha} - \langle\hat{c}^{\dagger}_{k+Q,\alpha'}\sigma^{z}_{\alpha'\alpha}\hat{c}_{k,\alpha}\rangle + \langle\hat{c}^{\dagger}_{k+Q,\alpha'}\sigma^{z}_{\alpha'\alpha}\hat{c}_{k,\alpha}\rangle\right)$
and $\hat{c}^{\dagger}_{k'+Q,\beta'}\sigma^{z}_{\beta'\beta}\hat{c}_{k',\beta}$ by $\left(\hat{c}^{\dagger}_{k'+Q,\beta'}\sigma^{z}_{\beta'\beta}\hat{c}_{k',\beta} - \langle\hat{c}^{\dagger}_{k'+Q,\beta'}\sigma^{z}_{\beta'\beta}\hat{c}_{k',\beta}\rangle + \langle\hat{c}^{\dagger}_{k'+Q,\beta'}\sigma^{z}_{\beta'\beta}\hat{c}_{k',\beta}\rangle\right)$ in eq.(3.1.2)

$$
\begin{aligned}
H_{SDW} = &-\sum_{k,k'}\sum_{\substack{\alpha,\alpha'\\,\beta,\beta'}}\frac{V^s}{2}\left(\hat{c}^{\dagger}_{k+Q,\alpha'}\sigma^{z}_{\alpha'\alpha}\hat{c}_{k,\alpha} - \langle\hat{c}^{\dagger}_{k+Q,\alpha'}\sigma^{z}_{\alpha'\alpha}\hat{c}_{k,\alpha}\rangle + \langle\hat{c}^{\dagger}_{k+Q,\alpha'}\sigma^{z}_{\alpha'\alpha}\hat{c}_{k,\alpha}\rangle\right)\\
&\times\left(\hat{c}^{\dagger}_{k'+Q,\beta'}\sigma^{z}_{\beta'\beta}\hat{c}_{k',\beta} - \langle\hat{c}^{\dagger}_{k'+Q,\beta'}\sigma^{z}_{\beta'\beta}\hat{c}_{k',\beta}\rangle + \langle\hat{c}^{\dagger}_{k'+Q,\beta'}\sigma^{z}_{\beta'\beta}\hat{c}_{k',\beta}\rangle\right)\\
= &-\sum_{k,k'}\sum_{\substack{\alpha,\alpha'\\,\beta,\beta'}}\frac{V^s}{2}\left(\hat{c}^{\dagger}_{k+Q,\alpha'}\sigma^{z}_{\alpha'\alpha}\hat{c}_{k,\alpha} - \langle\hat{c}^{\dagger}_{k+Q,\alpha'}\sigma^{z}_{\alpha'\alpha}\hat{c}_{k,\alpha}\rangle\right)\left(\hat{c}^{\dagger}_{k'+Q,\beta'}\sigma^{z}_{\beta'\beta}\hat{c}_{k',\beta}\right.\\
&\left.- \langle\hat{c}^{\dagger}_{k'+Q,\beta'}\sigma^{z}_{\beta'\beta}\hat{c}_{k',\beta}\rangle\right)\\
&+\left(\hat{c}^{\dagger}_{k+Q,\alpha'}\sigma^{z}_{\alpha'\alpha}\hat{c}_{k,\alpha} - \langle\hat{c}^{\dagger}_{k+Q,\alpha'}\sigma^{z}_{\alpha'\alpha}\hat{c}_{k,\alpha}\rangle\right)\langle\hat{c}^{\dagger}_{k'+Q,\beta'}\sigma^{z}_{\beta'\beta}\hat{c}_{k',\beta}\rangle\\
&+\langle\hat{c}^{\dagger}_{k+Q,\alpha'}\sigma^{z}_{\alpha'\alpha}\hat{c}_{k,\alpha}\rangle\left(\hat{c}^{\dagger}_{k'+Q,\beta'}\sigma^{z}_{\beta'\beta}\hat{c}_{k',\beta} - \langle\hat{c}^{\dagger}_{k'+Q,\beta'}\sigma^{z}_{\beta'\beta}\hat{c}_{k',\beta}\rangle\right)\\
&+\langle\hat{c}^{\dagger}_{k+Q,\alpha'}\sigma^{z}_{\alpha'\alpha}\hat{c}_{k,\alpha}\rangle\langle\hat{c}^{\dagger}_{k'+Q,\beta'}\sigma^{z}_{\beta'\beta}\hat{c}_{k',\beta}\rangle.
\end{aligned}
$$

The first term is a product of the fluctuation which is neglected. The last one is just a constant. Omitting this term, one obtains the mean field Hamiltonian

$$
\begin{aligned}
H_{SDW} = &-\sum_{k,k'}\sum_{\substack{\alpha,\alpha'\\,\beta,\beta'}}\frac{V^s}{2}\left(\hat{c}^{\dagger}_{k+Q,\alpha'}\sigma^{z}_{\alpha'\alpha}\hat{c}_{k,\alpha}\langle\hat{c}^{\dagger}_{k'+Q,\beta'}\sigma^{z}_{\beta'\beta}\hat{c}_{k',\beta}\rangle\right.\\
&\left.+\hat{c}^{\dagger}_{k'+Q,\beta'}\sigma^{z}_{\beta'\beta}\hat{c}_{k',\beta}\langle\hat{c}^{\dagger}_{k+Q,\alpha'}\sigma^{z}_{\alpha'\alpha}\hat{c}_{k,\alpha}\rangle\right).
\end{aligned}
$$

Exchanging of indices unprimed to primed in one of the term leads to the following equation

$$
H_{SDW} = -\sum_{k,k'}\sum_{\substack{\alpha,\alpha'\\,\beta,\beta'}}V^s\hat{c}^{\dagger}_{k+Q,\alpha'}\sigma^{z}_{\alpha'\alpha}\hat{c}_{k,\alpha}\langle\hat{c}^{\dagger}_{k'+Q,\beta'}\sigma^{z}_{\beta'\beta}\hat{c}_{k',\beta}\rangle.
$$

Let us introduce SDW gap

$$
\Delta_s = -V^s\sum_{k',\beta,\beta'}\langle\hat{c}^{\dagger}_{k'+Q,\beta'}\sigma^{z}_{\beta\beta'}\hat{c}_{k',\beta}\rangle \qquad (3.3)
$$

which is zero for normal state. This enables us to write mean field SDW Hamiltonian in the concise form

$$H_{SDW} = \Delta_s \sum_{k,\alpha,\alpha'} \hat{c}^{\dagger}_{k+Q,\alpha'} \sigma^{z}_{\alpha'\alpha} \hat{c}_{k,\alpha}. \quad (3.4)$$

Next, to obtain the CDW Hamiltonian, one insert the following interaction into the Hamiltonian eq.(3.1)

$$V^{DW}_{\alpha\alpha'\beta\beta'}(k, k', q) = \frac{V^c}{2} \delta(q - Q) \delta_{\alpha'\alpha} \delta_{\beta'\beta} . \quad (3.5)$$

One finds the CDW Hamiltonian

$$H_{CDW} = -\sum_{k,k'} \sum_{\alpha,\beta} \frac{V^c}{2} \hat{c}^{\dagger}_{k+Q,\alpha} \hat{c}_{k,\alpha} \hat{c}^{\dagger}_{k'+Q,\beta} \hat{c}_{k',\beta} \quad (3.6)$$

Again, we apply the mean field technique to eq.(3.6) and introduce CDW gap

$$\Delta_c = -\sum_{k',\beta} V^c \langle \hat{c}^{\dagger}_{k'+Q,\beta} \hat{c}_{k',\beta} \rangle. \quad (3.7)$$

Thus we obtain the mean field Hamiltonian of CDW

$$H_{CDW} = \Delta_c \sum_{k,\alpha} \hat{c}^{\dagger}_{k+Q,\alpha} \hat{c}_{k,\alpha} . \quad (3.8)$$

To see the meaning of SDW state, let us consider the case of SDW state; $\Delta_s \neq 0$

$$\sum_{k',\beta,\beta'} \langle \hat{c}^{\dagger}_{k'+Q,\beta'} \sigma^{z}_{\beta\beta'} \hat{c}_{k',\beta} \rangle = \sum_{k'} \left(\langle \hat{c}^{\dagger}_{k'+Q,\uparrow} \hat{c}_{k',\uparrow} \rangle - \langle \hat{c}^{\dagger}_{k'+Q,\downarrow} \hat{c}_{k',\downarrow} \rangle \right) \neq 0 \quad (3.9)$$

Consider the Fourier transform of the field operator

$$\hat{c}^{\dagger}_{k,\beta} = \frac{1}{\sqrt{N}} \sum_{i} e^{ik\cdot r_i} \hat{c}^{\dagger}_{i,\beta} \;\; ; \hat{c}^{\dagger}_{i,\beta} = \frac{1}{\sqrt{N}} \sum_{k} e^{-ik\cdot r_i} \hat{c}^{\dagger}_{k,\beta} \quad (3.10)$$

Where i, j are indexes of lattice sites. Inserting in 3.9, we get

$$0 \neq \sum_{k'} \left(\langle \hat{c}^{\dagger}_{k'+Q,\uparrow} \hat{c}_{k',\uparrow} \rangle - \langle \hat{c}^{\dagger}_{k'+Q,\downarrow} \hat{c}_{k',\downarrow} \rangle \right) = \sum_{i} e^{iQ\cdot r_i} \left(\langle \hat{c}^{\dagger}_{i,\uparrow} \hat{c}_{i,\uparrow} \rangle - \langle \hat{c}^{\dagger}_{i,\downarrow} \hat{c}_{i,\downarrow} \rangle \right)$$

This shows that there is a net spin density on lattice site and it varies from site to site. Similarly, for CDW state

$$0 \neq \sum_{k'} \left(\langle \hat{c}^{\dagger}_{k'+Q,\uparrow} \hat{c}_{k',\uparrow} \rangle + \langle \hat{c}^{\dagger}_{k'+Q,\downarrow} \hat{c}_{k',\downarrow} \rangle \right) = \sum_{i} e^{iQ\cdot r_i} \left(\langle \hat{c}^{\dagger}_{i,\uparrow} \hat{c}_{i,\uparrow} \rangle + \langle \hat{c}^{\dagger}_{i,\downarrow} \hat{c}_{i,\downarrow} \rangle \right)$$

there is net charge density on the position **r** and it varies as static wave with wave number Q.

The simple model Hamiltonian of the coexistence of SDW and CDW can be constructed by summing the mean field Hamiltonian of the relevant interaction together with the kinetic energy term

$$\mathrm{H} = \sum_{k,\alpha}(\varepsilon_k - \mu)\hat{c}^{\dagger}_{k,\alpha}\hat{c}_{k,\alpha} + \Delta_s \sum_{k,\alpha,\alpha'} \hat{c}^{\dagger}_{k+Q,\alpha'}\sigma^{z}_{\alpha'\alpha}\hat{c}_{k,\alpha} + \Delta_c \sum_{k,\alpha}\hat{c}^{\dagger}_{k+Q,\alpha}\hat{c}_{k,\alpha}\,. \qquad (3.11)$$

To write down this in the quadratic form, we expand the index of spin and the index k over the first Brillouin zone to the reduced Brillouin zone with the index (k),

$$\begin{aligned}\mathrm{H} = \sum_{(k)}(\varepsilon_k - \mu)\hat{c}^{\dagger}_{k,\uparrow}\hat{c}_{k,\uparrow} &+ (\varepsilon_{k+Q} - \mu)\hat{c}^{\dagger}_{k+Q,\uparrow}\hat{c}_{k+Q,\uparrow} + (\varepsilon_k - \mu)\hat{c}^{\dagger}_{k,\downarrow}\hat{c}_{k,\downarrow} \\ &+ (\varepsilon_{k+Q} - \mu)\hat{c}^{\dagger}_{k+Q,\downarrow}\hat{c}_{k+Q,\downarrow} + (\Delta_s + \Delta_c)\left(\hat{c}^{\dagger}_{k+Q,\uparrow}\hat{c}_{k,\uparrow} + \hat{c}^{\dagger}_{k,\uparrow}\hat{c}_{k+Q,\uparrow}\right) \\ &+ (\Delta_c - \Delta_s)\left(\hat{c}^{\dagger}_{k+Q,\downarrow}\hat{c}_{k,\downarrow} + \hat{c}^{\dagger}_{k,\downarrow}\hat{c}_{k+Q,\downarrow}\right).\end{aligned} \qquad (3.12)$$

This can be written in the matrix form

$$\begin{aligned}\mathrm{H} &= \Psi^{\dagger}_{\alpha}\mathbb{H}\Psi_{\alpha} \\ &= \sum_{(k)}\begin{pmatrix}\hat{c}^{\dagger}_{k,\uparrow} & \hat{c}^{\dagger}_{k+Q,\uparrow} & \hat{c}^{\dagger}_{k,\downarrow} & \hat{c}^{\dagger}_{k+Q,\downarrow}\end{pmatrix}\begin{pmatrix}\xi_k & (\Delta_s + \Delta_c) & 0 & 0 \\ (\Delta_s + \Delta_c) & \xi_{k+Q} & 0 & 0 \\ 0 & 0 & \xi_k & (\Delta_c - \Delta_s) \\ 0 & 0 & (\Delta_c - \Delta_s) & \xi_{k+Q}\end{pmatrix}\begin{pmatrix}\hat{c}_{k,\uparrow} \\ \hat{c}_{k+Q,\uparrow} \\ \hat{c}_{k,\downarrow} \\ \hat{c}_{k+Q,\downarrow}\end{pmatrix}\end{aligned}$$

where $\Psi^{\dagger}_{\alpha} = \begin{pmatrix}\hat{c}^{\dagger}_{k,\uparrow} & \hat{c}^{\dagger}_{k+Q,\uparrow} & \hat{c}^{\dagger}_{k,\downarrow} & \hat{c}^{\dagger}_{k+Q,\downarrow}\end{pmatrix}$ is a 4 components Numbu field operator and $\xi_k = (\varepsilon_k - \mu)$. Letting

$$\gamma_k = \frac{\xi_k - \xi_{k+Q}}{2} = \frac{\varepsilon_k - \varepsilon_{k+Q} - \mu + \mu}{2} = \frac{\varepsilon_k - \varepsilon_{k+Q}}{2}$$

$$\frac{\xi_k + \xi_{k+Q}}{2} = \frac{\varepsilon_k + \varepsilon_{k+Q} - \mu - \mu}{2} = \frac{\varepsilon_k + \varepsilon_{k+Q}}{2} = \frac{\varepsilon_k + \varepsilon_{k+Q}}{2} - \mu = \delta_k - \mu$$

the Hamiltonian matrix can be written as

$$\mathbb{H} = \begin{pmatrix}(\delta_k - \mu) + \gamma_k & (\Delta_s + \Delta_c) & 0 & 0 \\ (\Delta_s + \Delta_c) & (\delta_k - \mu) - \gamma_k & 0 & 0 \\ 0 & 0 & (\delta_k - \mu) + \gamma_k & (\Delta_c - \Delta_s) \\ 0 & 0 & (\Delta_c - \Delta_s) & (\delta_k - \mu) - \gamma_k\end{pmatrix}. \qquad (3.13)$$

Or in the term of Pauli matrices

$$\mathbb{H} = (\delta_k - \mu)\rho_o\sigma_o + \gamma_k\,\rho_o\sigma_3 + \Delta_c\rho_o\sigma_1 + \Delta_s\rho_3\sigma_1.$$

where $\rho_i\sigma_j$ is the 4x4 Pauli matrices. The eigenvalues of $\mathbb{H}$ are

$$E_1 = \delta_k - \mu - \sqrt{\gamma_k^2 + (\Delta_c - \Delta_s)^2};\ E_2 = \delta_k - \mu + \sqrt{\gamma_k^2 + (\Delta_c - \Delta_s)^2}$$
$$E_3 = \delta_k - \mu - \sqrt{\gamma_k^2 + (\Delta_c + \Delta_s)^2};\ E_4 = \delta_k - \mu + \sqrt{\gamma_k^2 + (\Delta_c + \Delta_s)^2} \quad (3.14)$$

which are often called the energy of a quasi particle. For our calculation we suppose that the energy dispersion is given by the tight binding model. According to the Tight binding method the energy of conduction electron for 2 D square lattice is

$$\varepsilon_k = 2t_o(\cos k_x + \cos k_y) + t_1 \cos k_x \cos k_y + t_2(\cos 2k_x + \cos 2k_y) + \cdots \quad (3.15)$$

Assuming that all hopping integrals t_i vanish except $t_0 \neq 0$, then the energy bands of the electron are

$$\varepsilon_k = 2t_o(\cos k_x + \cos k_y) \quad (3.16)$$

with the following relations

$$\varepsilon_{-k} = \varepsilon_k;\ \varepsilon_{k+Q} = -\varepsilon_k;\ \varepsilon_{-k-Q} = \varepsilon_{k+Q} = -\varepsilon_k\ . \quad (3.17)$$

Fermi surface and the dispersion curve of eq.(3.16) are shown in figure 18. This Fermi surface is called perfect nesting, every points on Fermi surface can be connected to that on the opposite by a nesting vector Q=(π, π).

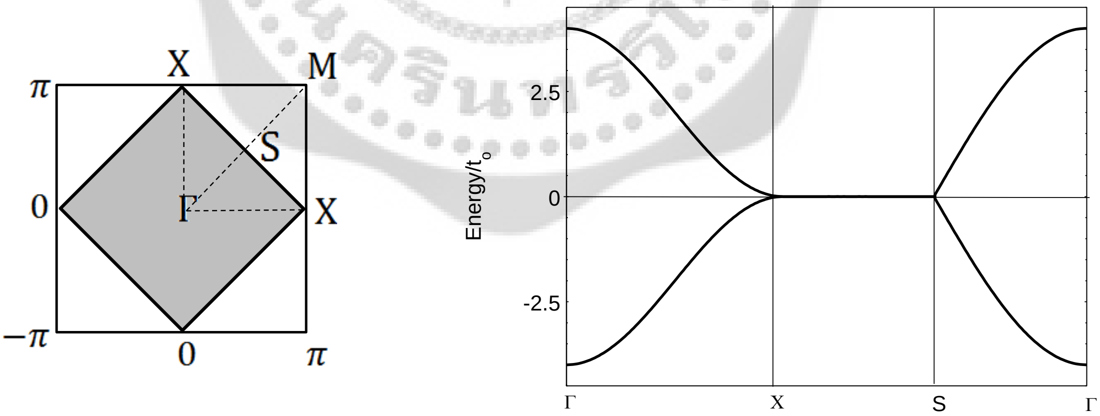


Figure 18 Fermi surface and dispersion curve along ΓXSΓ for eq.(3.16)

The width of the energy band is $2W = \varepsilon_{0,0} - \varepsilon_{\pi,\pi} = 8t_o$. If the chemical potential is fixed to be zero and together with eq.(3.17) the Hamiltonian matrix and their eigenvalues reduce to

$$\mathbb{H} = \begin{pmatrix} \varepsilon_k & (\Delta_s + \Delta_c) & 0 & 0 \\ (\Delta_s + \Delta_c) & -\varepsilon_k & 0 & 0 \\ 0 & 0 & \varepsilon_k & (\Delta_c - \Delta_s) \\ 0 & 0 & (\Delta_c - \Delta_s) & -\varepsilon_k \end{pmatrix} \tag{3.18}$$

and

$$\begin{gathered} E_1 = -\sqrt{\varepsilon_k^2 + (\Delta_c - \Delta_s)^2};\;\; E_2 = \sqrt{\varepsilon_k^2 + (\Delta_c - \Delta_s)^2} \\ E_3 = -\sqrt{\varepsilon_k^2 + (\Delta_c + \Delta_s)^2};\;\; E_4 = \sqrt{\varepsilon_k^2 + (\Delta_c + \Delta_s)^2}\,. \end{gathered} \tag{3.19}$$

2 Gap Equations

In this section the gap equations will be derived from eq.(3.18) using Green's function technique. The one particle Green's function is defined as an average of the product of the field operator over the ensemble

$$\mathbb{G}(k,\tau) = -\langle T_\tau \Psi_k(\tau)\Psi_k^\dagger(0)\rangle\,. \tag{3.20}$$

Here T_τ is a time order operator, it order the operator in such a way that the time argument of the operator decrease from left to right. Substituting the following expression into eq.(3.20)

$$\begin{aligned} \Psi_k(\tau)\Psi_k^\dagger(0) &= \begin{pmatrix} \hat{c}_{k,\uparrow} \\ \hat{c}_{k+Q,\uparrow} \\ \hat{c}_{k,\downarrow} \\ \hat{c}_{k+Q,\downarrow} \end{pmatrix} \begin{pmatrix} \hat{c}^\dagger_{k,\uparrow} & \hat{c}^\dagger_{k+Q,\uparrow} & \hat{c}^\dagger_{k,\downarrow} & \hat{c}^\dagger_{k+Q,\downarrow} \end{pmatrix} \\ &= \begin{pmatrix} \hat{c}_{k,\uparrow}\hat{c}^\dagger_{k,\uparrow} & \hat{c}_{k,\uparrow}\hat{c}^\dagger_{k+Q,\uparrow} & \hat{c}_{k,\uparrow}\hat{c}^\dagger_{k,\downarrow} & \hat{c}_{k,\uparrow}\hat{c}^\dagger_{k+Q,\downarrow} \\ \hat{c}_{k+Q,\uparrow}\hat{c}^\dagger_{k,\uparrow} & \hat{c}_{k+Q,\uparrow}\hat{c}^\dagger_{k+Q,\uparrow} & \hat{c}_{k+Q,\uparrow}\hat{c}^\dagger_{k,\downarrow} & \hat{c}_{k+Q,\uparrow}\hat{c}^\dagger_{k+Q,\downarrow} \\ \hat{c}_{k,\downarrow}\hat{c}^\dagger_{k,\uparrow} & \hat{c}_{k,\downarrow}\hat{c}^\dagger_{k+Q,\uparrow} & \hat{c}_{k,\downarrow}\hat{c}^\dagger_{k,\downarrow} & \hat{c}_{k,\downarrow}\hat{c}^\dagger_{k+Q,\downarrow} \\ \hat{c}_{k+Q,\downarrow}\hat{c}^\dagger_{k,\uparrow} & \hat{c}_{k+Q,\downarrow}\hat{c}^\dagger_{k+Q,\uparrow} & \hat{c}_{k+Q,\downarrow}\hat{c}^\dagger_{k,\downarrow} & \hat{c}_{k+Q,\downarrow}\hat{c}^\dagger_{k+Q,\downarrow} \end{pmatrix} \end{aligned}$$

we obtain the matrix of Green's function

$$\begin{aligned} &\mathbb{G}(k,\tau) \\ &= -\begin{pmatrix} \langle T_\tau\hat{c}_{k,\uparrow}\hat{c}^\dagger_{k,\uparrow}\rangle & \langle T_\tau\hat{c}_{k,\uparrow}\hat{c}^\dagger_{k+Q,\uparrow}\rangle & \langle T_\tau\hat{c}_{k,\uparrow}\hat{c}^\dagger_{k,\downarrow}\rangle & \langle T_\tau\hat{c}_{k,\uparrow}\hat{c}^\dagger_{k+Q,\downarrow}\rangle \\ \langle T_\tau\hat{c}_{k+Q,\uparrow}\hat{c}^\dagger_{k,\uparrow}\rangle & \langle T_\tau\hat{c}_{k+Q,\uparrow}\hat{c}^\dagger_{k+Q,\uparrow}\rangle & \langle T_\tau\hat{c}_{k+Q,\uparrow}\hat{c}^\dagger_{k,\downarrow}\rangle & \langle T_\tau\hat{c}_{k+Q,\uparrow}\hat{c}^\dagger_{k+Q,\downarrow}\rangle \\ \langle T_\tau\hat{c}_{k,\downarrow}\hat{c}^\dagger_{k,\uparrow}\rangle & \langle T_\tau\hat{c}_{k,\downarrow}\hat{c}^\dagger_{k+Q,\uparrow}\rangle & \langle T_\tau\hat{c}_{k,\downarrow}\hat{c}^\dagger_{k,\downarrow}\rangle & \langle T_\tau\hat{c}_{k,\downarrow}\hat{c}^\dagger_{k+Q,\downarrow}\rangle \\ \langle T_\tau\hat{c}_{k+Q,\downarrow}\hat{c}^\dagger_{k,\uparrow}\rangle & \langle T_\tau\hat{c}_{k+Q,\downarrow}\hat{c}^\dagger_{k+Q,\uparrow}\rangle & \langle T_\tau\hat{c}_{k+Q,\downarrow}\hat{c}^\dagger_{k,\downarrow}\rangle & \langle T_\tau\hat{c}_{k+Q,\downarrow}\hat{c}^\dagger_{k+Q,\downarrow}\rangle \end{pmatrix}. \end{aligned} \tag{3.21}$$

However, it is more convenient to analyze the frequency domain Greens function $\mathbb{G}(k, i\omega_n)$ instead. The time domain Greens function can be obtained from the frequency domain via the Fourier series

$$\mathbb{G}(k,\tau) = \frac{1}{\beta}\lim_{\tau\to 0}\sum_{n} e^{-i\omega_n\tau}\,\mathbb{G}(k, i\omega_n)$$

where $\omega_n = (2n+1)\pi T$ is a Mutsubara frequency. From eq.(3. 18) $\mathbb{G}(k, i\omega_n)$ can be determined from

$$\mathbb{G}(k, i\omega_n) = (i\omega_n - \mathbb{H})^{-1}\,. \tag{3.22}$$

After some calculation, we get the non-vanishing components of frequency domain Greens function as following

$$\begin{aligned}
\mathbb{G}_{1,1}(k, i\omega_n) &= -\langle T_\tau \hat{c}_{k,\uparrow}\hat{c}^\dagger_{k,\uparrow}\rangle_{\omega_n} = \frac{i\omega_n + \varepsilon_k}{(i\omega_n - E_3)(i\omega_n - E_4)},\\
\mathbb{G}_{1,2}(k, i\omega_n) &= -\langle T_\tau \hat{c}_{k,\uparrow}\hat{c}^\dagger_{k+Q,\uparrow}\rangle_{\omega_n} = \frac{(\Delta_c + \Delta_s)}{(i\omega_n - E_3)(i\omega_n - E_4)} = \mathbb{G}_{2,1}(k, i\omega_n)\\
&= -\langle T_\tau \hat{c}_{k+Q,\uparrow}\hat{c}^\dagger_{k,\uparrow}\rangle_{\omega_n},\\
\mathbb{G}_{2,2}(k, i\omega_n) &= -\langle T_\tau \hat{c}_{k+Q,\uparrow}\hat{c}^\dagger_{k+Q,\uparrow}\rangle_{\omega_n} = \frac{i\omega_n - \varepsilon_k}{(i\omega_n - E_3)(i\omega_n - E_4)},\\
\mathbb{G}_{3,3}(k, i\omega_n) &= -\langle T_\tau \hat{c}_{k,\downarrow}\hat{c}^\dagger_{k,\downarrow}\rangle_{\omega_n} = \frac{i\omega_n + \varepsilon_k}{(i\omega_n - E_1)(i\omega_n - E_2)},\\
\mathbb{G}_{3,4}(k, i\omega_n) &= -\langle T_\tau \hat{c}_{k,\downarrow}\hat{c}^\dagger_{k+Q,\downarrow}\rangle_{\omega_n} = \frac{(\Delta_c - \Delta_s)}{(i\omega_n - E_1)(i\omega_n - E_2)} = \mathbb{G}_{4,3}(k, i\omega_n)\\
&= -\langle T_\tau \hat{c}_{k+Q,\downarrow}\hat{c}^\dagger_{k,\downarrow}\rangle_{\omega_n},\\
\mathbb{G}_{4,4}(k, i\omega_n) &= -\langle T_\tau \hat{c}_{k+Q,\downarrow}\hat{c}^\dagger_{k+Q,\downarrow}\rangle_{\omega_n} = \frac{i\omega_n - \varepsilon_k}{(i\omega_n - E_1)(i\omega_n - E_2)}\,.
\end{aligned}$$

Rewrite in the matrix form

$$\mathbb{G}(k, i\omega_n) = \begin{pmatrix}
\frac{i\omega + \varepsilon_k}{(i\omega - E_3)(i\omega - E_4)} & \frac{(\Delta_c + \Delta_s)}{(i\omega - E_3)(i\omega - E_4)} & & \\
\frac{(\Delta_c + \Delta_s)}{(i\omega - E_3)(i\omega - E_4)} & \frac{i\omega - \varepsilon_k}{(i\omega - E_3)(i\omega - E_4)} & & \\
 & & \frac{i\omega + \varepsilon_k}{(i\omega - E_1)(i\omega - E_2)} & \frac{(\Delta_c - \Delta_s)}{(i\omega - E_1)(i\omega - E_2)} \\
 & & \frac{(\Delta_c - \Delta_s)}{(i\omega - E_1)(i\omega - E_2)} & \frac{i\omega - \varepsilon_k}{(i\omega - E_1)(i\omega - E_2)}
\end{pmatrix}. \tag{3.23}$$

This can be rewritten in term of sub matrices

$$\mathbb{G} = \begin{pmatrix} \mathbb{G}_1 & 0 \\ 0 & \mathbb{G}_2 \end{pmatrix} \tag{3.24}$$

where

$$\mathbb{G}_1 = \frac{1}{(i\omega - E_3)(i\omega - E_4)}\begin{pmatrix} i\omega + \varepsilon_k & (\Delta_c + \Delta_s) \\ (\Delta_c + \Delta_s) & i\omega - \varepsilon_k \end{pmatrix}$$
$$= \frac{i\omega\tau_o + \varepsilon_k\,\tau_3 + (\Delta_c + \Delta_s)\tau_1}{(i\omega - E_3)(i\omega - E_4)},$$

$$\mathbb{G}_2 = \frac{1}{(i\omega - E_1)(i\omega - E_2)}\begin{pmatrix} i\omega + \varepsilon_k & (\Delta_c - \Delta_s) \\ (\Delta_c - \Delta_s) & i\omega - \varepsilon_k \end{pmatrix} \qquad (3.25)$$
$$= \frac{i\omega\tau_o + \gamma_k\,\tau_3 + (\Delta_c - \Delta_s)\tau_1}{(i\omega - E_1)(i\omega - E_2)},$$

$$\tau_o = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \tau_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \tau_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Next, we consider the component of Green's function which are related to the SDW and CDW gap, $\mathbb{G}_{1,2}(k,\tau)$ and $\mathbb{G}_{3,4}(k,\tau)$.

$$\mathbb{G}_{1,2}(k,\tau) = \mathbb{G}_{2,1}(k,\tau) = \frac{1}{\beta}\lim_{\tau\to 0}\sum_n e^{-i\omega_n\tau}\,\mathbb{G}_{1,2}(k,i\omega_n)$$
$$= \frac{1}{\beta}\lim_{\tau\to 0}\sum_n e^{-i\omega_n\tau}\frac{(\Delta_c + \Delta_s)}{(i\omega_n - E_3)(i\omega_n - E_4)}$$
$$\mathbb{G}_{3,4}(k,\tau) = \mathbb{G}_{4,3}(k,\tau) = \frac{1}{\beta}\lim_{\tau\to 0}\sum_n e^{-i\omega_n\tau}\,\mathbb{G}_{3,4}(k,i\omega_n)$$
$$= \frac{1}{\beta}\lim_{\tau\to 0}\sum_n e^{-i\omega_n\tau}\frac{(\Delta_c - \Delta_s)}{(i\omega_n - E_1)(i\omega_n - E_2)}$$

To obtain the time domain Greens function we use the Matsubara frequency sum rule for simple pole

$$T\sum_n g(i\omega_n)e^{-i\omega_n\tau} = \sum_i \mathrm{Rez}\big(g(z_j)\big)\,f(z_j)e^{z_j\tau}, \quad f(z_j) \text{ is Fermi function.} \qquad (3.26)$$

Applying the sum rule to $\mathbb{G}_{1,2}(k,\tau)$ and $\mathbb{G}_{3,4}(k,\tau)$, we have

$$\mathbb{G}_{1,2}(k,\tau) = \frac{(\Delta_c + \Delta_s)}{2\sqrt{\varepsilon_k^2 + \Delta_+^2}}\big(f(E_4) - f(E_3)\big),$$
$$\mathbb{G}_{3,4}(k,\tau) = \frac{(\Delta_c - \Delta_s)}{2\sqrt{\gamma_k^2 + \Delta_-^2}}\big(f(E_2) - f(E_1)\big). \qquad (3.27)$$

The CDW gap eq.(3.7) can be expressed in term of Green's function by

$$\Delta_c = -V^c\sum_{k'}\langle \hat{c}^\dagger_{k'+Q,\uparrow}\hat{c}_{k',\uparrow}\rangle + \langle \hat{c}^\dagger_{k'+Q,\downarrow}\hat{c}_{k',\downarrow}\rangle = -V^c\sum_{k'}\mathbb{G}_{1,2} + \mathbb{G}_{3,4}\,.$$

From eq.(3.27) one finds

$$\Delta_c = -\frac{V^s}{2}\sum_k \left\{\frac{\Delta_+\big(f(E_4) - f(E_3)\big)}{\sqrt{\varepsilon_k^2 + \Delta_+^2}} - \frac{\Delta_-\big(f(E_2) - f(E_1)\big)}{\sqrt{\varepsilon_k^2 + \Delta_-^2}}\right\}.$$

By using of the following relations

$$f[x] - f[-x] = -\mathrm{Tanh}\left(\frac{\beta x}{2}\right)$$

we find

$$\Delta_c = \frac{V^c}{2}\sum_k \left\{\frac{\Delta_+}{\sqrt{\varepsilon_k^2 + \Delta_+^2}}\mathrm{Tanh}\left(\frac{\sqrt{\varepsilon_k^2 + \Delta_+^2}}{2T}\right) - \frac{\Delta_-}{\sqrt{\varepsilon_k^2 + \Delta_-^2}}\mathrm{Tanh}\left(\frac{\sqrt{\varepsilon_k^2 + \Delta_-^2}}{2T}\right)\right\} \qquad (3.28)$$

where $(\Delta_c + \Delta_s) = \Delta_+, (\Delta_s - \Delta_c) = \Delta_-$.Using the same process the SDW gap is given by

$$\Delta_s = -V^s \sum_k \mathbb{G}_{1,2}(k,\tau) - \mathbb{G}_{3,4}(k,\tau)$$

$$= \frac{V^s}{2}\sum_k \left\{\frac{\Delta_+}{\sqrt{\varepsilon_k^2 + \Delta_+^2}}\mathrm{Tanh}\left(\frac{\sqrt{\varepsilon_k^2 + \Delta_+^2}}{2T}\right) + \frac{\Delta_-}{\sqrt{\varepsilon_k^2 + \Delta_-^2}}\mathrm{Tanh}\left(\frac{\sqrt{\varepsilon_k^2 + \Delta_-^2}}{2T}\right)\right\}. \qquad (3.29)$$

3 Density of States

In this part the density of state (DOS) will be derived from Green's function. Rewrite the denominator in eq.(3.25) as

$$\frac{1}{(i\omega - E_3)(i\omega - E_4)} = \frac{1}{(E_4 - E_3)}\left(\frac{1}{(i\omega - E_4)} - \frac{1}{(i\omega - E_3)}\right),$$
$$\frac{1}{(i\omega - E_1)(i\omega - E_2)} = \frac{1}{(E_2 - E_1)}\left(\frac{1}{(i\omega - E_2)} - \frac{1}{(i\omega - E_1)}\right).$$

These two expressions enable us to write the sub matrix Green's function as

$$\begin{aligned}\mathbb{G}_1 &= \left(\frac{1}{(i\omega - E_4)} - \frac{1}{(i\omega - E_3)}\right)\frac{i\omega\tau_o + \varepsilon_k\,\tau_3 + (\Delta_c + \Delta_s)\tau_1}{(E_4 - E_3)},\\ \mathbb{G}_2 &= \left(\frac{1}{(i\omega - E_2)} - \frac{1}{(i\omega - E_1)}\right)\frac{i\omega\tau_o + \varepsilon_k\,\tau_3 + (\Delta_c - \Delta_s)\tau_1}{(E_2 - E_1)}.\end{aligned} \qquad (3.30)$$

The spectral function can be directly calculated from retarded Green function as

$$\mathbb{A}(\mathrm{k},\omega) = -\frac{1}{\pi}\mathrm{Im}\,\mathbb{G}^{\mathrm{R}}(\mathrm{k},\omega). \tag{3.31}$$

The retarded Green function can be obtained by analytic continuation of the imaginary time Green function to the real axis from the upper half plane,

$$\mathbb{G}^{\mathrm{R}}(\mathrm{k},\omega) = \mathbb{G}(\mathrm{k},\mathrm{i}\omega)|_{\mathrm{i}\omega\to\omega+\mathrm{i}0^+}, \tag{3.32}$$

where 0+ denotes a positive infinitesimal number. From eq.(3.30) we can get the 11 component of $\mathbb{G}^{\mathrm{R}}$

$$\mathbb{G}^{\mathrm{R}}_{11} = \frac{\omega + \mathrm{i}0^+ + \varepsilon_{\mathrm{k}}}{(\mathrm{E}_4 - \mathrm{E}_3)}\left(\frac{\omega - \mathrm{E}_4 - \mathrm{i}0^+}{(\omega - \mathrm{E}_4)^2 + (0^+)^2} - \frac{\omega - \mathrm{E}_3 - \mathrm{i}0^+}{(\omega - \mathrm{E}_3)^2 + (0^+)^2}\right).$$

Its imaginary part is

$$\mathrm{Im}\mathbb{G}^{\mathrm{R}}_{11} = \frac{1}{(\mathrm{E}_4 - \mathrm{E}_3)}\left(\frac{(-\varepsilon_{\mathrm{k}} - \mathrm{E}_4)0^+}{(\omega - \mathrm{E}_4)^2 + (0^+)^2} - \frac{(-\varepsilon_{\mathrm{k}} - \mathrm{E}_3)0^+}{(\omega - \mathrm{E}_3)^2 + (0^+)^2}\right).$$

Applying the following identity to above equation

$$\delta(\mathrm{k}) = \lim_{\tau\to0+}\frac{1}{\pi}\frac{\tau}{\tau^2 + \mathrm{k}^2},$$

thus $\mathrm{Im}\mathbb{G}_{11}$ takes the form

$$\mathrm{Im}\mathbb{G}^{\mathrm{R}}_{11}(\mathrm{k},\omega)$$
$$= \frac{\pi}{2\sqrt{\varepsilon_{\mathrm{k}}^2 + \Delta_+^2}}\left((-\varepsilon_{\mathrm{k}} - \sqrt{\varepsilon_{\mathrm{k}}^2 + \Delta_+^2})\delta(\omega - \sqrt{\varepsilon_{\mathrm{k}}^2 + \Delta_+^2}) - (-\varepsilon_{\mathrm{k}} + \sqrt{\varepsilon_{\mathrm{k}}^2 + \Delta_+^2})\delta(\omega + \sqrt{\varepsilon_{\mathrm{k}}^2 + \Delta_+^2})\right)$$

Using the following property of Dirac delta function

$$\delta(\mathrm{g}(\mathrm{x})) = \sum_i \frac{\delta(\mathrm{x} - \mathrm{x_i})}{|\mathrm{g}'(\mathrm{x_i})|};\, \mathrm{g}(\mathrm{x_i}) = 0,$$

for positive ω

$$\delta\left(\omega - \sqrt{\varepsilon^2 + \Delta_+^2}\right) = \frac{\omega}{\sqrt{\omega^2 - \Delta_+^2}}\left(\delta\left(\varepsilon - \sqrt{\omega^2 - \Delta_+^2}\right) + \delta\left(\varepsilon + \sqrt{\omega^2 - \Delta_+^2}\right)\right),$$

and for negative ω

$$\delta\left(-|\omega| + \sqrt{\varepsilon_{\mathrm{k}}^2 + \Delta_+^2}\right) = \frac{|\omega|}{\sqrt{\omega^2 - \Delta_+^2}}\left(\delta\left(\varepsilon - \sqrt{\omega^2 - \Delta_+^2}\right) + \delta\left(\varepsilon + \sqrt{\omega^2 - \Delta_+^2}\right)\right).$$

So that, we have

$$
\begin{aligned}
&\mathrm{Im}\mathbb{G}_{11}^{\mathrm{R}}(\mathrm{k},\omega) \\
&= \frac{\pi}{2\sqrt{\varepsilon_{\mathrm{k}}^2+\Delta_+^2}}\left[\left(-\varepsilon_{\mathrm{k}}-\sqrt{\varepsilon_{\mathrm{k}}^2+\Delta_+^2}\right)\frac{\omega}{\sqrt{\omega^2-\Delta_+^2}}\left(\delta\left(\varepsilon-\sqrt{\omega^2-\Delta_+^2}\right)+\delta\left(\varepsilon+\sqrt{\omega^2-\Delta_+^2}\right)\right)\right. \\
&\qquad\left.+\left(-\varepsilon_{\mathrm{k}}+\sqrt{\varepsilon_{\mathrm{k}}^2+\Delta_+^2}\right)\frac{|\omega|}{\sqrt{\omega^2-\Delta_+^2}}\delta\left(\varepsilon-\sqrt{\omega^2-\Delta_+^2}\right)+\delta\left(\varepsilon+\sqrt{\omega^2-\Delta_+^2}\right)\right]
\end{aligned}
$$

Next we calculate $\mathrm{Im}\mathbb{G}_{11}(\omega)=\sum_k \mathrm{Im}\mathbb{G}_{11}(\mathrm{k},\omega)$ by changing the summation to integration over the band width with the constant DOS, N(0)

$$
\mathrm{Im}\mathbb{G}_{11}(\omega)=\mathrm{N}(0)\int_{-\mathrm{W}}^{\mathrm{W}} d\varepsilon\, \mathrm{Im}\mathbb{G}_{11}(\mathrm{k},\omega).
$$

After some calculation and rearrangement, we have

$$
\mathrm{Im}\mathbb{G}_{11}^{\mathrm{R}}(\omega)=-\mathrm{N}(0)\frac{|\omega|}{\sqrt{\omega^2-\Delta_+^2}}\theta(\omega-\Delta_+).
$$

The remaining components can be calculated using the same procedure. Therefore, the diagonal elements of spectral function are

$$
\begin{aligned}
\mathbb{A}_{11}(\omega)=\mathbb{A}_{22}(\omega)&=\mathrm{N}(0)\frac{|\omega|}{\sqrt{\omega^2-\Delta_+^2}}\theta(|\omega|-\Delta_+), \\
\mathbb{A}_{33}(\omega)=\mathbb{A}_{44}(\omega)&=\mathrm{N}(0)\frac{|\omega|}{\sqrt{\omega^2-\Delta_-^2}}\theta(-\omega)\theta(|\omega|-\Delta_-).
\end{aligned}
\tag{3.33}
$$

The density of state calculated from the spectral function is

$$
\begin{aligned}
\rho(\omega)&=\mathrm{Tr}\mathbb{A}(\omega) \\
&=2\mathrm{N}(0)\left[\frac{|\omega|}{\sqrt{\omega^2-\Delta_+^2}}\theta(-\omega)\theta(|\omega|-\Delta_+)\right. \\
&\qquad\left.+\frac{|\omega|}{\sqrt{\omega^2-\Delta_-^2}}\theta(-\omega)\theta(|\omega|-\Delta_-)\right].
\end{aligned}
\tag{3.34}
$$

4 Free Energy

The free energy is defined by

$$
\Omega=\mathrm{U}-\mathrm{TS}-\mu\mathrm{N}=\langle \mathrm{H}_{\mathrm{grand}}\rangle-\mathrm{TS}\,, \tag{3.35}
$$

where S is entropy.

$$S = -\sum_i f(E_i)\ln\big(f(E_i)\big) + \big(1 - f(E_i)\big)\ln\big(1 - f(E_i)\big), \tag{3.36}$$

where the sum runs over all microstates and $f(E_i)$ is the Fermi function.
Using the following relation

$$f(E)\ln\big(f(E)\big) + \big(1 - f(E)\big)\ln\big(1 - f(E)\big) = \frac{\beta E}{2}\big(1 - 2f(E_i)\big) - \ln(2) - \ln\left(\mathrm{Cosh}\left(\frac{\beta E}{2}\right)\right),$$

the entropy can be written as

$$S = -\sum_{k,i}\left(\frac{\beta E_i}{2}\big(1 - 2f(E_i)\big) - \ln\left(2\mathrm{Cosh}\left(\frac{\beta E_i}{2}\right)\right)\right). \tag{3.37}$$

Next we consider an average of the grand canonical Hamiltonian

$$\langle H_{grand}\rangle = \sum_{k,\alpha}\varepsilon_k\langle\hat{c}^\dagger_{k,\alpha}\hat{c}_{k,\alpha}\rangle - \frac{\Delta_s}{V^s}\sum_{k,\alpha,\alpha'}\langle -V^s\hat{c}^\dagger_{k+Q,\alpha'}\sigma^z_{\alpha'\alpha}\hat{c}_{k,\alpha}\rangle - \frac{\Delta_c}{V^c}\sum_{k,\alpha}\langle -V^c\hat{c}^\dagger_{k+Q,\alpha}\hat{c}_{k,\alpha}\rangle.$$

From eq.(3.3) and (3.7) one finds

$$\langle H_{grand}\rangle = \sum_{k,\alpha}\varepsilon_k\langle\hat{c}^\dagger_{k,\alpha}\hat{c}_{k,\alpha}\rangle - \frac{\Delta_s^2}{V^s} - \frac{\Delta_c^2}{V^c}. \tag{3.38}$$

The first term can be represented by Green's function as

$$\sum_{k,\alpha}\varepsilon_k\langle\hat{c}^\dagger_{k,\alpha}\hat{c}_{k,\alpha}\rangle = \sum_k\varepsilon_k\big(\langle\hat{c}^\dagger_{k,\uparrow}\hat{c}_{k,\uparrow}\rangle + \langle\hat{c}^\dagger_{k,\downarrow}\hat{c}_{k,\downarrow}\rangle\big) = \sum_k\varepsilon_k\big(\mathbb{G}_{1,1} + \mathbb{G}_{3,3}\big). \tag{3.39}$$

After using the Matsubara sum rule $\mathbb{G}_{1,1}$ and $\mathbb{G}_{3,3}$ are

$$\mathbb{G}_{1,1}(k,\tau) = \frac{E^+ - \varepsilon_k}{E^+}f(E_3) + \frac{\varepsilon_k + E^+}{E^+}f(E_4)\,,$$
$$\mathbb{G}_{3,3}(k,\tau) = \frac{E^- - \varepsilon_k}{E^-}f(E_1) + \frac{\varepsilon_k + E^-}{E^-}f(E_2)\,,$$

where $E^\pm = \sqrt{\varepsilon_k^2 + \Delta_\pm^2}$. Substitution $\mathbb{G}_{1,1}$ and $\mathbb{G}_{3,3}$ in eq.(3.39) yields

$$\sum_{k,\alpha}\varepsilon_k\langle\hat{c}^\dagger_{k,\alpha}\hat{c}_{k,\alpha}\rangle = \sum_k\left(\frac{\varepsilon_k E^+ - \varepsilon_k^2}{E^+}f(E_3) + \frac{\varepsilon_k^2 + \varepsilon_k E^+}{E^+}f(E_4) + \frac{\varepsilon_k E^- - \varepsilon_k^2}{E^-}f(E_1) + \frac{\varepsilon_k^2 + \varepsilon_k E^-}{E^-}f(E_2)\right).$$

In this expression E_is are even funcion while ε_k is odd function under the change $k \to k + Q$. It is clearly seen that if one change the summation over k to summation over (k) the term ε_k will be cancle out by ε_{k+Q} ,thus

$$\sum_{k,\alpha} \varepsilon_k \langle \hat{c}^{\dagger}_{k,\alpha} \hat{c}_{k,\alpha} \rangle = \sum_{k} \left(\frac{-\varepsilon_k^2}{E^+} f(E_3) + \frac{\varepsilon_k^2}{E^+} f(E_4) + \frac{-\varepsilon_k^2}{E^-} f(E_1) + \frac{\varepsilon_k^2}{E^-} f(E_2) \right). \qquad (3.40)$$

Substituting eqs.(3.37), (3.38) and (3.40) to eq.(3.35), we arrive at

$$\Omega = -\frac{\Delta_s^2}{V^s} - \frac{\Delta_c^2}{V^c} + \sum_{k} \left(\frac{\Delta_+^2}{E^+} \mathrm{Tanh}\left(\frac{E^+}{2T}\right) + \frac{\Delta_-^2}{E^-} \mathrm{Tanh}\left(\frac{E^-}{2T}\right) \right) - T \sum_{k,i} \ln\left(2\mathrm{Cosh}\left(\frac{\beta E_i}{2}\right) \right).$$

From eqs.(3.28) and (3.29) the third term can be written in term of SDW and CDW gap

$$\begin{aligned} &\sum_{k} \left(\frac{\Delta_+^2}{\sqrt{+}} \mathrm{Tanh}\left(\frac{\sqrt{+}}{2T}\right) + \frac{\Delta_-^2}{\sqrt{-}} \mathrm{Tanh}\left(\frac{\sqrt{+}}{2T}\right) \right) \\ &\qquad = \Delta_s \sum_{k} \left(\frac{\Delta_+}{\sqrt{+}} \mathrm{Tanh}\left(\frac{\sqrt{+}}{2T}\right) + \frac{\Delta_-}{\sqrt{-}} \mathrm{Tanh}\left(\frac{\sqrt{+}}{2T}\right) \right) \\ &\qquad + \Delta_c \sum_{k} \left(\frac{\Delta_+}{\sqrt{+}} \mathrm{Tanh}\left(\frac{\sqrt{+}}{2T}\right) - \frac{\Delta_-}{\sqrt{-}} \mathrm{Tanh}\left(\frac{\sqrt{+}}{2T}\right) \right) = \frac{2\Delta_s^2}{V^s} + \frac{2\Delta_c^2}{V^c}. \end{aligned}$$

Finally we obtaine the free energy for coexistence phase

$$\Omega_{coex} = \frac{\Delta_s^2}{V^s} + \frac{\Delta_c^2}{V^c} - 2T \sum_{k} \ln\left(2\mathrm{Cosh}\left(\frac{E_4}{2T}\right) \right) + \ln\left(2\mathrm{Cosh}\left(\frac{E_2}{2T}\right) \right). \qquad (3.41)$$

Minimizing this free energy with respet to Δ_c and Δ_s we will get the gap equations eq.(3.28) and (3.29) respectively.For normal state putting $\Delta_s, \Delta_c = 0$ in eq.(3.41) we get the free energy of normal state

$$\Omega_n = -4T \sum_{k} \ln\left(2\mathrm{Cosh}\left(\frac{\varepsilon_k}{2T}\right) \right).$$

The free energy difference is

$$\begin{aligned} \delta\Omega &= \Omega_{coex} - \Omega_n \\ &= \frac{\Delta_s^2}{V^s} + \frac{\Delta_c^2}{V^c} - 2T \sum_{k} \left(\ln\left(\frac{\mathrm{Cosh}(E_4/2T)}{\mathrm{Cosh}(\varepsilon_k/2T)} \right) + \ln\left(\frac{\mathrm{Cosh}(E_2/2T)}{\mathrm{Cosh}(\varepsilon_k/2T)} \right) \right). \end{aligned} \qquad (3.42)$$

5 Pure SDW and CDW State

By setting $\Delta_c = 0$ in eq.(3.29) we obtain the gap equation for pure SDW

$$\frac{1}{V^s} = \sum_k \frac{1}{\sqrt{\varepsilon_k^2 + \Delta_s^2}} \mathrm{Tanh}\left(\frac{\sqrt{\varepsilon_k^2 + \Delta_s^2}}{2T}\right) \tag{3.43}$$

Similarly, the gap equation of pure CDW takes the same form as pure SDW

$$\frac{1}{V^c} = \sum_k \frac{1}{\sqrt{\varepsilon_k^2 + \Delta_c^2}} \mathrm{Tanh}\left(\frac{\sqrt{\varepsilon_k^2 + \Delta_c^2}}{2T}\right) \tag{3.44}$$

The results of the study of pure CDW are certainly identical to pure SDW. Firstly, we will consider the zero temperature gap of SDW with constant DOS N(0). At zero temperature if $W \gg \Delta_s$ the gap equation of SDW is

$$\frac{1}{V^s} = \sum_k \frac{1}{\sqrt{\varepsilon_k^2 + \Delta_s^2}} = 2N(0)\int_0^W \frac{d\varepsilon}{\sqrt{\varepsilon^2 + \Delta_s^2}} \approx 2N(0)\ln\left(\frac{2W}{\Delta_s(0)}\right)$$

Leting $N(0)V^s = g_s$, we have

$$\frac{1}{2g_s} = \ln\left(\frac{2W}{\Delta_s(0)}\right). \tag{3.45}$$

The zero-temperature gap is

$$\Delta_s(0) = 2We^{-\frac{1}{2g_s}}. \tag{3.46}$$

Next the critical temperature for pure SDW T_{so} is evaluated using standard BCS technique. From gap equation eq.(3.43) we put $\Delta_s = 0$ and then convert the summation to integration over the band width

$$\frac{1}{V^s} = \sum_k \frac{1}{\sqrt{\varepsilon_k^2 + \Delta_s^2}} \mathrm{Tanh}\left(\frac{1}{2T}\sqrt{\varepsilon_k^2 + \Delta_s^2}\right) \rightarrow \frac{1}{2g} = \int_0^W d\varepsilon \frac{1}{\varepsilon} \mathrm{Tanh}\left(\frac{\varepsilon}{2T_c}\right) = \int_0^{W/2T_{so}} \frac{1}{x}\mathrm{Tanh}(x)\, dx.$$

Using integration by part technique with an assumption that $W/2T_{so} \gg 1$, we get

$$\frac{1}{2g} = \mathrm{Log}\left(\frac{2\gamma W}{\pi T_{so}}\right). \tag{3.47}$$

The critical temperature is

$$T_{so} = \frac{2\gamma}{\pi} W e^{-1/2g} \cong 1.44 W e^{-1/2g}. \tag{3.48}$$

The gap-to-T_c ratio is same as BCS theory

$$\frac{2\Delta_s(0)}{T_{so}} = \frac{4We^{-1/2g}}{\frac{2\gamma}{\pi}We^{-1/2g}} = \frac{2\pi}{\gamma} \cong 3.52. \tag{3.49}$$

Using the same technique as BCS we have near critical temperature gap

$$\Delta_s^2(T_{so}) = \frac{8\pi^2}{7\xi(3)} T_{so}(T_{so} - T) \ . \tag{3.50}$$

We also have the specific heat

$$c_{SDW}(T) = \frac{4N(0)}{T^2} \int_0^W d\varepsilon \frac{e^{\sqrt{\varepsilon^2+\Delta_s^2}/T}}{\left(e^{\sqrt{\varepsilon^2+\Delta_s^2}/T} + 1\right)^2} \left(\varepsilon^2 + \Delta_s^2 - \frac{T}{2}\frac{d\Delta_s^2}{dT}\right). \tag{3.51}$$

At the critical temperature one finds

$$c_{SDW}(T_{so}) = \frac{4N(0)}{T_{so}^2} \int_0^W d\varepsilon \frac{e^{\varepsilon/T_{so}}}{(e^{\varepsilon/T_{so}} + 1)^2} \left(\varepsilon^2 + T_{so}^2 \frac{4\pi^2}{7\xi(3)}\right). \tag{3.52}$$

And we get the specific heat jump at the critical temperature

$$\frac{\Delta c}{c_n} = \frac{c_{SDW} - c_n}{c_n} = \frac{12}{7\xi(3)} = 1.426 \ .$$

This result is identical to the typical value of the BCS theory.

6 Zero-Temperature Gaps

At zero temperature eqs.(3.28) and (3.29) take the form

$$\Delta_s = \frac{V^s}{2}\sum_k\left(\frac{\Delta_+}{\sqrt{\varepsilon_k^2+\Delta_+^2}}+\frac{\Delta_-}{\sqrt{\varepsilon_k^2+\Delta_-^2}}\right),$$

$$\Delta_c = \frac{V^c}{2}\sum_k\left(\frac{\Delta_+}{\sqrt{\varepsilon_k^2+\Delta_+^2}}-\frac{\Delta_-}{\sqrt{\varepsilon_k^2+\Delta_-^2}}\right). \tag{3.53}$$

Changing the summation to integration over band width and introducing the notation of coupling constant $g_s = N(0)V^s, g_c = N(0)V^c$, one finds

$$\Delta_s = g_s\left(\Delta_+\ln\left(\frac{W+\sqrt{W^2+\Delta_+^2}}{|\Delta_+|}\right)+\Delta_-\ln\left(\frac{E_c+\sqrt{E_c^2+\Delta_-^2}}{|\Delta_-|}\right)\right),$$

$$\Delta_c = g_c\left(\Delta_+\ln\left(\frac{W+\sqrt{W^2+\Delta_+^2}}{|\Delta_+|}\right)-\Delta_-\ln\left(\frac{W+\sqrt{W^2+\Delta_-^2}}{|\Delta_-|}\right)\right).$$

If $W \gg \Delta_c, \Delta_s$, the gaps equation can be approximated. And after rearranging the equation,we get

$$\frac{1}{g_s} = \left(1+\frac{\Delta_c}{\Delta_s}\right)\ln\left(\frac{2W}{|\Delta_+|}\right)+\left(1-\frac{\Delta_c}{\Delta_s}\right)\ln\left(\frac{2W}{|\Delta_-|}\right)$$

$$\frac{1}{g_c} = \left(\frac{\Delta_s}{\Delta_c}+1\right)\ln\left(\frac{2W}{|\Delta_+|}\right)-\left(\frac{\Delta_s}{\Delta_c}-1\right)\ln\left(\frac{2W}{|\Delta_-|}\right) \tag{3.54}$$

After some rearrangement we get

$$\frac{1}{g_s} = \ln\left(\frac{4W^2}{\Delta_s^2\left|1+\frac{\Delta_c}{\Delta_s}\right|^{1+\frac{\Delta_c}{\Delta_s}}\left|1-\frac{\Delta_c}{\Delta_s}\right|^{1-\frac{\Delta_c}{\Delta_s}}}\right);\frac{1}{g_c} = \ln\left(\frac{4W^2}{\Delta_c^2}\frac{\left|\frac{\Delta_s}{\Delta_c}-1\right|^{\frac{\Delta_s}{\Delta_c}-1}}{\left|\frac{\Delta_s}{\Delta_c}+1\right|^{1+\frac{\Delta_s}{\Delta_c}}}\right)$$

Let $\Delta_s(0)/\Delta_c(0) = a$ that give

$$\frac{1}{g_s} = \ln\left(\frac{4W^2}{\Delta_s^2\left|\frac{a+1}{a}\right|^{\frac{a+1}{a}}\left|\frac{a-1}{a}\right|^{\frac{a-1}{a}}}\right); \frac{1}{g_c} = \ln\left(\frac{4W^2}{\Delta_c^2}\frac{|a-1|^{a-1}}{|a+1|^{1+a}}\right)$$

Finally, we obtain the gap at zero temperature of SDW and CDW

$$\Delta_s(0) = \frac{2We^{-1/2g_s}}{\sqrt{\left|\frac{a+1}{a}\right|^{\frac{a+1}{a}}\left|\frac{a-1}{a}\right|^{\frac{a-1}{a}}}} \tag{3.55}$$

$$\Delta_c(0) = 2We^{-1/2g_c}\sqrt{\frac{|a-1|^{a-1}}{|a+1|^{1+a}}} \tag{3.56}$$

7 Critical Temperature

The non-zero-temperature gaps are given by

$$\Delta_s = g_s\int_0^W d\varepsilon\left(\frac{\Delta_+}{\sqrt{\varepsilon^2+\Delta_+^2}}\mathrm{Tanh}\left(\frac{\sqrt{\varepsilon^2+\Delta_+^2}}{2T}\right) + \frac{\Delta_-}{\sqrt{\varepsilon^2+\Delta_-^2}}\mathrm{Tanh}\left(\frac{\sqrt{\varepsilon^2+\Delta_-^2}}{2T}\right)\right) \tag{3.57}$$

$$\Delta_c = g_c\int_0^W d\varepsilon\left(\frac{\Delta_+}{\sqrt{\varepsilon^2+\Delta_+^2}}\mathrm{Tanh}\left(\frac{\sqrt{\varepsilon^2+\Delta_+^2}}{2T}\right) - \frac{\Delta_-}{\sqrt{\varepsilon^2+\Delta_-^2}}\mathrm{Tanh}\left(\frac{\sqrt{\varepsilon^2+\Delta_-^2}}{2T}\right)\right) \tag{3.58}$$

To study this two couple equations the difficulty is that it is impossible to analytically solve this couple equations. However,we can study these equation by simplify them under the under the appropriate approximation conditions. To obtain the analytic expression of the critical temperature, we will derive the integration formula approximately and then apply it to eq.(3.57) and (3.58) at the critical temperature. We start by considering the following integral

$$\int_0^W \frac{d\varepsilon}{\sqrt{\varepsilon^2+\Delta_i^2}}\mathrm{Tanh}\left(\frac{\sqrt{\varepsilon^2+\Delta_i^2}}{2T}\right). \tag{3.59}$$

Using the following relation

$$\frac{\mathrm{Tanh}(x)}{x} = \sum_{n=0}\frac{2}{x^2+(\pi(n+1/2))^2},$$

the integrand in eq.(3.59) can be expressed as

$$\frac{1}{\sqrt{\varepsilon^2+\Delta_i^2}}\mathrm{Tanh}\left(\frac{1}{2T}\sqrt{\varepsilon^2+\Delta_i^2}\right)=4T\sum_n\frac{1}{\varepsilon^2+\Delta_i^2+\omega_n^2}\,;\omega=(2n+1)\pi T.$$

We expand the denominator using geometric series

$$\frac{1}{\varepsilon^2+\Delta_i^2+\omega_n^2}=\frac{1}{(\varepsilon^2+\omega_n^2)\left(1+\frac{\Delta_i^2}{\varepsilon^2+\omega_n^2}\right)}=\sum_m(-1)^m\frac{\Delta_i^{2m}}{(\varepsilon^2+\omega_n^2)^{m+1}}.$$

This expansion is valid for $\Delta_i/\pi T<1$. This is the first our approximation condition. Therefore, eq.(3.59) becomes

$$\int_0^W\frac{d\varepsilon}{\sqrt{\varepsilon^2+\Delta_i^2}}\mathrm{Tanh}\left(\frac{\sqrt{\varepsilon^2+\Delta_i^2}}{2T}\right)$$
$$=4T\left[\int_0^W\sum_{n=0}\frac{d\varepsilon}{\varepsilon^2+\omega_n^2}+\sum_{n=0}\sum_{m=1}(-1)^m\,\Delta_i^{2m}\int_0^W\frac{d\varepsilon}{(\varepsilon^2+\omega_n^2)^{m+1}}\right]\quad(3.60)$$

We calculate the first term on the right side using the standard method of BCS theory with the second approximation condition $W\gg T$,

$$4T\int_0^W\sum_{n=0}\frac{d\varepsilon}{\varepsilon^2+\omega_n^2}=\int_0^W\frac{\mathrm{Tanh}(\varepsilon/2T)}{\varepsilon}d\varepsilon=\ln\left(\frac{2\gamma W}{\pi T}\right).\quad(3.61)$$

Next, we consider the second term using the variable $x=\varepsilon/\omega_n$

$$4T\sum_{n=0}\sum_{m=1}(-1)^m\,\Delta_i^{2m}\int_0^E\frac{d\varepsilon}{(\varepsilon^2+\omega_n^2)^{m+1}}=4T\sum_{n=0}\sum_{m=1}(-1)^m\,\frac{\Delta_i^{2m}}{\omega_n^{2m+1}}\int_0^{E/\omega_n}\frac{dx}{(1+x^2)^{m+1}}$$

Consider the formula

$$\int_0^{\frac{W}{\omega_n}} \frac{dx}{(1+x^2)^{m+1}} = \left(\frac{(W/\omega_n)}{2m+1} \sum_{k=1}^{m} \frac{(2m+1)(2m-1)(2m-3)\ldots(2m-2k+3)}{2^k(m)(m-1)(m-2)\ldots(m-k+1)\left(1+\left(\frac{W}{\omega_n}\right)^2\right)^{m-k+1}} + \frac{(2m-1)!!}{2^m m!} \mathrm{ArcTan}\left(\frac{W}{\omega_n}\right) \right).$$

For $W \gg T$, this can be approximate as

$$\int_0^{W/\omega_n} \frac{dx}{(1+x^2)^{m+1}} \approx \frac{(2m-1)!!}{2^m m!} \frac{\pi}{2}.$$

Thus we obtain

$$4T \sum_{n=0} \sum_{m=1} (-1)^m \Delta_i^{2m} \int_0^W \frac{d\varepsilon}{(\varepsilon^2+\omega_n^2)^{m+1}} = 2 \sum_{m=1} (-1)^m \left(\sum_{n=0} \frac{1}{(2n+1)^{2m+1}} \right) \frac{(2m-1)!!}{\pi^{2m} 2^m m!} (\beta\Delta_i)^{2m},$$

$$= 2 \sum_{m=1} (-1)^m \left(1 - \frac{1}{2^{2m+1}}\right) \frac{\xi(2m+1)(2m-1)!!}{\pi^{2m} 2^m m!} (\beta\Delta_i)^{2m}, \quad (3.62)$$

here $\xi(2m+1)$ stands for the Riemann zeta function and $\beta = 1/T$. From eq.(3.61) and (3.62) together with eq.(3.60) we can get the formula

$$\int_0^W \frac{d\varepsilon}{\sqrt{\varepsilon^2+\Delta_i^2}} \mathrm{Tanh}\left(\frac{\sqrt{\varepsilon^2+\Delta_i^2}}{2T} \right) = \ln\left(\frac{2\gamma W}{\pi T}\right) + 2 \sum_{m=1} B_m \left(\frac{\beta\Delta_i}{\pi}\right)^{2m}, \quad (3.63)$$

Here $B_m = (-1)^m \left(1 - \frac{1}{2^{2m+1}}\right) \frac{\xi(2m+1)(2m-1)!!}{2^m m!}$,

or in a short form

$$\int_0^W \frac{d\varepsilon}{\sqrt{\varepsilon^2+\Delta_i^2}} \mathrm{Tanh}\left(\frac{\sqrt{\varepsilon^2+\Delta_i^2}}{2T} \right) = \ln\left(\frac{2\gamma W}{\pi T}\right) + 2 \sum_{m=1} [\Delta_i].$$

Applying this formula to eq.(3.57) and (3.58), we have

$$\frac{1}{g_s} = \left(1 + \frac{\Delta_c}{\Delta_s}\right)\left(\ln\left(\frac{2\gamma W}{\pi T}\right) + 2 \sum_{m=1} [\Delta_+]\right) + \left(1 - \frac{\Delta_c}{\Delta_s}\right)\left(\ln\left(\frac{2\gamma W}{\pi T}\right) + 2 \sum_{m=1} [\Delta_-]\right),$$

$$\frac{1}{g_c} = \left(1+\frac{\Delta_s}{\Delta_c}\right)\left(\ln\left(\frac{2\gamma W}{\pi T}\right)+2\sum_{m=1}[\Delta_+]\right)+\left(1-\frac{\Delta_s}{\Delta_c}\right)\left(\ln\left(\frac{2\gamma W}{\pi T}\right)+2\sum_{m=1}[\Delta_-]\right).$$

After some rearrangement and use of the binomial expansion, $(a+b)^m = \sum_{j=0} C_j^m a^{m-j} b^j$, we obtain the gap equations

$$\begin{aligned}\frac{1}{2g_s} = \ln\left(\frac{2\gamma W}{\pi T}\right) &+ 2\sum_{m=1} B_m \left\{\left(\frac{\beta}{\pi}\right)^{2m} (C_0^{2m}\Delta_c^{2m} + C_2^{2m}\Delta_c^{2m-2}\Delta_s^2 \ldots + C_{2m}^{2m}\Delta_s^{2m})\right\} \\ &+ 2\sum_{m=1} B_m \left\{\left(\frac{\beta}{\pi}\right)^{2m} (C_1^{2m}\Delta_c^{2m} + C_3^{2m}\Delta_c^{2m-2}\Delta_s^2 \ldots \right. \\ &\left. + C_{2m-1}^{2m}\Delta_c^2\Delta_s^{2m-2})\right\},\end{aligned} \tag{3.64}$$

$$\begin{aligned}\frac{1}{2g_c} = \ln\left(\frac{2\gamma W}{\pi T}\right) &+ 2\sum_{m=1} B_m \left\{\left(\frac{\beta}{\pi}\right)^{2m} (C_0^{2m}\Delta_c^{2m} + C_2^{2m}\Delta_c^{2m-2}\Delta_s^2 \ldots + C_{2m}^{2m}\Delta_s^{2m})\right\} \\ &+ 2\sum_{m=1} B_m \left\{\left(\frac{\beta}{\pi}\right)^{2m} (C_1^{2m}\Delta_c^{2m-2}\Delta_s^2 + C_3^{2m}\Delta_c^{2m-4}\Delta_s^4 \ldots \right. \\ &\left. + C_{2m-1}^{2m}\Delta_s^{2m})\right\}.\end{aligned} \tag{3.65}$$

These two equations are a crucial starting point in the study of the SDW and CDW critical temperature and the specific heat. In order to determined the critical temperature we separate the study into 2 cases; $T_c > T_s$ and $T_c < T_s$

Case 1. $T_c > T_s$ At T_s, putting $\Delta_s = 0$ in eq.(3.27) and (3.28) the gap equations become

$$\frac{1}{2g_s} = \ln\left(\frac{2\gamma W}{\pi T_s}\right) + 2\sum_{m=1} B_m\,(2m+1)\left(\frac{\Delta_c}{\pi T_s}\right)^{2m}, \tag{3.66}$$

$$\frac{1}{2g_c} = \ln\left(\frac{2\gamma W}{\pi T_s}\right) + 2\sum_{m=1} B_m \left(\frac{\Delta_c}{\pi T_s}\right)^{2m}. \tag{3.67}$$

Subtracting eq.(3.66) from (3.67) and adding eq.(3.66) to (3.67), we arrive at

$$\left(\frac{1}{2g_c} - \frac{1}{2g_s}\right) = -4\sum_{m=1} B_m\, m\left(\frac{\Delta_c}{\pi T_s}\right)^{2m}, \tag{3.68}$$

$$\left(\frac{1}{2g_c} + \frac{1}{2g_s}\right) = 2\ln\left(\frac{2\gamma W}{\pi T_s}\right) + 4\sum_{m=1} B_m\,(m+1)\left(\frac{\Delta_c}{\pi T_s}\right)^{2m}. \tag{3.69}$$

From eq.(3.69) the critical temperature can be expressed as

$$T_s = \frac{2\gamma W}{\pi}\mathrm{Exp}\left(-\frac{1}{2}\left(\frac{1}{2g_c}+\frac{1}{2g_s}\right) + 2\sum_{m=1} B_m\,(m+1)\left(\frac{\Delta_c}{\pi T_s}\right)^{2m}\right). \tag{3.70}$$

This shows that by solving for ratio Δ_c/T_s in eq.(3.68) and substituting in eq.(3.70) the critical temperature can be calculated.

At T_c , setting $\Delta_c = 0$ in eq.(3.67) we get the ciritical temperature of pure CDW state

$$\frac{1}{2g_c} = \ln\left(\frac{2\gamma W}{\pi T_c}\right) \rightarrow T_c = \frac{2\gamma W}{\pi} e^{-1/2g_c}. \tag{3.71}$$

Case 2. $T_c < T_s$ Similar to the previous case, at T_c we get the following expression

$$\left(\frac{1}{2g_s} - \frac{1}{2g_c}\right) = -4\sum_{m=1} B_m\, m \left(\frac{\Delta_s}{\pi T_c}\right)^{2m}, \tag{3.72}$$

$$T_c = \frac{2\gamma W}{\pi} \mathrm{Exp}\left[-\frac{1}{2}\left(\frac{1}{2g_c} + \frac{1}{2g_s}\right) + 2\sum_{m=1} B_m\,(m+1)\left(\frac{\Delta_s}{\pi T_c}\right)^{2m}\right]. \tag{3.73}$$

At T_s we have

$$T_s = \frac{2\gamma W}{\pi} e^{-1/2g_s}. \tag{3.74}$$

8 Near Zero-Temperature Gaps

At near zero temperature the tanh() can be approximate as

$$\mathrm{Tanh}\left(\frac{\sqrt{\varepsilon_k^2 + \Delta_\pm^2}}{2T}\right) \approx 1 - 2e^{-\sqrt{\varepsilon_k^2+\Delta_\pm^2}/T}.$$

Inserting this expression into the gap equations eq.(3.2.9) and (3.2.10), we obtain

$$\frac{\Delta_s}{g_s} = \Delta_+ \ln\left(\frac{2W}{|\Delta_+|}\right) + \Delta_- \ln\left(\frac{2W}{|\Delta_-|}\right) - 2\Delta_+ \int_0^{W/\Delta_+} dx \frac{e^{-\frac{\Delta_+}{T}\sqrt{x^2+1}}}{\sqrt{x^2+1}} - 2\Delta_- \int_0^{W/\Delta_-} dx \frac{e^{-\frac{|\Delta_-|}{T}\sqrt{x^2+1}}}{\sqrt{x^2+1}}$$

$$\frac{\Delta_c}{g_c} = \Delta_+ \ln\left(\frac{2W}{|\Delta_+|}\right) - \Delta_- \ln\left(\frac{2W}{|\Delta_-|}\right) - 2\Delta_+ \int_0^{W/\Delta_+} dx \frac{e^{-\frac{\Delta_+}{T}\sqrt{x^2+1}}}{\sqrt{x^2+1}} + 2\Delta_- \int_0^{W/\Delta_-} dx \frac{e^{-\frac{|\Delta_-|}{T}\sqrt{x^2+1}}}{\sqrt{x^2+1}}$$

The remaining integral is exponentially small at low temperature, we introduce the new variable $y = \sqrt{x^2+1}$ and take the upper limit to infinity

$$\frac{\Delta_s}{g_s} = \Delta_+ \ln\left(\frac{2W}{|\Delta_+|}\right) + \Delta_- \ln\left(\frac{2W}{|\Delta_-|}\right) - 2\Delta_+ \int_1^{\infty} dy \frac{e^{-\frac{\Delta_+ y}{T}}}{\sqrt{y^2-1}} - 2\Delta_- \int_1^{\infty} dy \frac{e^{-\frac{|\Delta_-|y}{T}}}{\sqrt{y^2-1}}$$

$$\frac{\Delta_c}{g_c} = \Delta_+ \ln\left(\frac{2W}{|\Delta_+|}\right) - \Delta_- \ln\left(\frac{2W}{|\Delta_-|}\right) - 2\Delta_+ \int_1^\infty dy \frac{e^{-\frac{\Delta_+ y}{T}}}{\sqrt{y^2-1}} + 2\Delta_- \int_1^\infty dy \frac{e^{-\frac{|\Delta_-| y}{T}}}{\sqrt{y^2-1}}$$

The remaining integral can be represented by the modified Bessel function of the second kind

$$\frac{\Delta_s}{g_s} = \Delta_+ \ln\left(\frac{2W}{|\Delta_+|}\right) + \Delta_- \ln\left(\frac{2W}{|\Delta_-|}\right) - 2\Delta_+ K_0\left(\frac{\Delta_+}{T}\right) - 2\Delta_- K_0\left(\frac{|\Delta_-|}{T}\right)$$
$$\frac{\Delta_c}{g_c} = \Delta_+ \ln\left(\frac{2W}{|\Delta_+|}\right) - \Delta_- \ln\left(\frac{2W}{|\Delta_-|}\right) - 2\Delta_+ K_0\left(\frac{\Delta_+}{T}\right) + 2\Delta_- K_0\left(\frac{|\Delta_-|}{T}\right)$$

Applying the asymptotic expansion

$$K_\nu(z) = \sqrt{\frac{\pi}{2z}} e^{-z} \left(1 - \frac{(4\nu^2 - 1^2)}{8z} + \frac{(4\nu^2 - 1^2)(4\nu^2 - 3^2)}{2!\,(8z)^2} + \cdots\right)$$
$$K_0(z) \approx \sqrt{\frac{\pi}{2z}} e^{-z}$$

we have

$$\frac{1}{g_s} = \frac{\Delta_+(T)}{\Delta_s(T)} \ln\left(\frac{2W}{|\Delta_+(T)|}\right) + \frac{\Delta_-(T)}{\Delta_s(T)} \ln\left(\frac{2W}{|\Delta_-(T)|}\right) - \frac{\Delta_+(T)}{\Delta_s(T)} e^{-\frac{\Delta_+(T)}{T}} \sqrt{\frac{2T\pi}{\Delta_+(T)}} - \frac{\Delta_-(T)}{\Delta_s(T)} e^{-\frac{|\Delta_-(T)|}{T}} \sqrt{\frac{2T\pi}{|\Delta_-(T)|}}$$
$$\frac{1}{g_c} = \frac{\Delta_+(T)}{\Delta_c(T)} \ln\left(\frac{2W}{|\Delta_+(T)|}\right) - \frac{\Delta_-(T)}{\Delta_c(T)} \ln\left(\frac{2W}{|\Delta_-(T)|}\right) - \frac{\Delta_+(T)}{\Delta_c(T)} e^{-\frac{\Delta_+(T)}{T}} \sqrt{\frac{2T\pi}{2\Delta_+(T)}} + \frac{\Delta_-(T)}{\Delta_c(T)} e^{-\frac{|\Delta_-(T)|}{T}} \sqrt{\frac{2T\pi}{|\Delta_-(T)|}}$$

where we have introduce $\Delta_i(T) = \Delta_i(0) + \delta\Delta_i(T)$. Then we get

$$\begin{aligned} &\frac{\Delta_s(0)}{g_s} + \frac{\Delta_c(0)}{g_c} + \frac{\delta\Delta_s(T)}{g_s} + \frac{\delta\Delta_c(T)}{g_c} \\ &\qquad = 2\big(\Delta_+(0) + \delta\Delta_+(T)\big) \mathrm{Log}\left[\frac{2W}{|\Delta_+(0) + \delta\Delta_+(T)|}\right] - 2\Delta_+(T) e^{-\frac{\Delta_+(T)}{T}} \sqrt{\frac{2T\pi}{\Delta_+(T)}}, \end{aligned} \tag{3.75}$$

$$\begin{aligned} &\frac{\Delta_s(0)}{g_s} - \frac{\Delta_c(0)}{g_c} + \frac{\delta\Delta_s(T)}{g_s} - \frac{\delta\Delta_c(T)}{g_c} \\ &\qquad = 2\big(\Delta_-(0) + \delta\Delta_-(T)\big) \mathrm{Log}\left[\frac{2W}{|\Delta_-(0) + \delta\Delta_-(T)|}\right] - 2\Delta_-(T) e^{-\frac{|\Delta_-(T)|}{T}} \sqrt{\frac{2T\pi}{|\Delta_-(T)|}} \end{aligned} \tag{3.76}$$

From the zero gap eq.(3.54), we have

$$\begin{aligned} \frac{\Delta_s(0)}{g_s} + \frac{\Delta_c(0)}{g_c} &= 2\Delta_+(0) \ln\left(\frac{2W}{|\Delta_+(0)|}\right), \\ \frac{\Delta_s(0)}{g_s} - \frac{\Delta_c(0)}{g_c} &= 2\Delta_-(0) \ln\left(\frac{2W}{|\Delta_-(0)|}\right). \end{aligned} \tag{3.77}$$

Inserting these to the left side of eq.(3.75) and (3.76), one finds that

$$\delta\Delta_+(\mathrm{T}) + \Delta_+(\mathrm{T})e^{-\frac{\Delta_+(\mathrm{T})}{\mathrm{T}}}\sqrt{\frac{2\mathrm{T}\pi}{\Delta_+(\mathrm{T})}} = \delta\Delta_+(\mathrm{T})\mathrm{Log}\left[\frac{2\mathrm{W}}{\Delta_+(\mathrm{T})}\right] - \frac{\delta\Delta_s(\mathrm{T})}{2g_s} - \frac{\delta\Delta_c(\mathrm{T})}{2g_c},$$
$$\delta\Delta_-(\mathrm{T}) + \Delta_-(\mathrm{T})e^{-\frac{|\Delta_-(\mathrm{T})|}{\mathrm{T}}}\sqrt{\frac{2\mathrm{T}\pi}{|\Delta_-(\mathrm{T})|}} = \delta\Delta_-(\mathrm{T})\mathrm{Log}\left[\frac{2\mathrm{W}}{|\Delta_-(\mathrm{T})|}\right] - \frac{\delta\Delta_s(\mathrm{T})}{2g_s} + \frac{\delta\Delta_c(\mathrm{T})}{2g_c},$$

where we have used the approximation for small x, $\mathrm{Log}[1 + x] \approx x$. From eq.(3.77) their right hand side is negligibly zero, thus we obtain the near zero temperature gaps

$$\Delta_+(\mathrm{T}) = \Delta_+(0) - e^{-\frac{\Delta_+(\mathrm{T})}{\mathrm{T}}}\sqrt{2\mathrm{T}\pi\Delta_+(0)}\,,$$
$$\Delta_-(\mathrm{T}) = \Delta_-(0) - e^{-\frac{|\Delta_-(\mathrm{T})|}{\mathrm{T}}}\sqrt{2\mathrm{T}\pi|\Delta_-(0)|}\,, \tag{3.78}$$

9 Near Critical Temperature Gaps

Assuming that $T_c > T_s$, at T_s from eq.(3.64) and (3.65) we have

$$\frac{1}{2g_s} + \frac{1}{2g_c} = 2\ln\left(\frac{2\gamma W}{\pi T_s}\right) + 2\sum_{m=1} B_m\,(2m+2)\left(\frac{\Delta_c}{\pi T_s}\right)^{2m} \tag{3.79}$$

In the vicinity of T_s , we retain only the term containing Δ_s^2

$$\frac{1}{2g_s} + \frac{1}{2g_c} = 2\ln\left(\frac{2\gamma W}{\pi T}\right) + 2\sum_{m=1} B_m\left((2m+2)\left(\frac{\Delta_c}{\pi T}\right)^{2m} + \frac{2m(2m+1)(m+1)}{3}\frac{\Delta_c^{2m-2}\Delta_s^2}{(\pi T)^{2m}}\right) \tag{3.80}$$

Equating eq.(3.79) and (3.80) , we find

$$2\ln\left(\frac{2\gamma W}{\pi T_s}\right) + 2\sum_{m=1} B_m\,(2m+2)\left(\frac{\Delta_c}{\pi T_s}\right)^{2m} = 2\ln\left(\frac{2\gamma W}{\pi T}\right) + 2\sum_{m=1} B_m\left((2m+2)\left(\frac{\Delta_c}{\pi T}\right)^{2m} + \frac{2m(2m+1)(m+1)}{3}\frac{\Delta_c^{2m-2}\Delta_s^2}{(\pi T)^{2m}}\right),$$

which can be written

$$\frac{T - T_s}{T_s} = \sum_{m=1} B_m\left((2m+2)\left\langle\left(\frac{\Delta_c}{\pi T}\right)^{2m} - \left(\frac{\Delta_c}{\pi T_s}\right)^{2m}\right\rangle + \frac{2m(2m+1)(m+1)}{3}\left(\frac{\Delta_c}{\pi T}\right)^{2m-2}\frac{\Delta_s^2}{(\pi T)^2}\right).$$

When $T \to T_s$ the first term in the parenthesis is negligibly small, thus we have the near T_s gap is

$$\Delta_s^2 = \frac{T_s(T - T_s)}{\sum_{m=1} B_m \frac{2m(2m+1)(m+1)}{3\pi^2}\left(\frac{\Delta_c}{\pi T_s}\right)^{2m-2}},$$

or

$$\Delta_s^2 = \frac{8\pi^2}{7\xi(3)}\frac{T_s(T_s - T)}{(2 - X)} \tag{3.81}$$

,where

$$X = \frac{8\pi^2}{7\xi(3)}\sum_{m=2} B_m \frac{2m(2m+1)(m+1)}{3\pi^2}\left(\frac{\Delta_c}{\pi T_s}\right)^{2m-2}. \tag{3.82}$$

Above T_s the system is pure CDW state, according to eq.(3.50) the near T_c gap read as

$$\Delta_c^2(T) = \frac{8\pi^2}{7\xi(3)} T_c(T_c - T). \tag{3.83}$$

10 Specific Heat

10.1 Specific Heat at Near Critical Temperature

According to the Fermi gas model the entropy of the coexistence of SDW and CDW is given by

$$S = -\sum_{k,i=1,2,3,4} f(E_i)\mathrm{Log}[f(E_i)] + \left(1 - f(E_i)\right)\mathrm{Log}[1 - f(E_i)]$$

, which can be written as

$$= -2\sum_{k,i=2,4} f(E_i)\mathrm{Log}[f(E_i)] + \left(1 - f(E_i)\right)\mathrm{Log}[1 - f(E_i)]$$

,where we have use the fact that $E_1 = -E_2, E_3 = -E_4$ .The specific heat derived from the entropy is

$$C = T\frac{dS}{dT} = T\frac{\partial S}{\partial f(E_i)}\frac{df(E_i)}{dT} = \frac{2}{T^2}\sum_{k,i=2,4}\frac{e^{E_i/T}}{(e^{E_i/T}+1)^2}\left(E_i^2 - E_i T\frac{dE_i}{dT}\right) \tag{3.84}$$

Assuming that $T_c > T_s$. Below the T_s the specific heat is

$$c = \frac{4N(0)}{T^2}\int_0^W d\varepsilon \left(\frac{e^{\sqrt{\varepsilon^2+\Delta_+^2}/T}}{\left(e^{\sqrt{\varepsilon^2+\Delta_+^2}/T}+1\right)^2}\left(\varepsilon^2+\Delta_s^2+\Delta_c^2+2\Delta_s\Delta_c-\frac{T}{2}\left(\frac{d}{dT}\Delta_s^2+\frac{d}{dT}2\Delta_s\Delta_c+\frac{d}{dT}\Delta_c^2\right)\right) + \frac{e^{\sqrt{\varepsilon^2+\Delta_-^2}/T}}{\left(e^{\sqrt{\varepsilon^2+\Delta_-^2}/T}+1\right)^2}\left(\varepsilon^2+\Delta_s^2+\Delta_c^2-2\Delta_s\Delta_c-\frac{T}{2}\left(\frac{d}{dT}\Delta_s^2-\frac{d}{dT}2\Delta_s\Delta_c+\frac{d}{dT}\Delta_c^2\right)\right)\right). \tag{3.85}$$

At T_s the specific heat of coexistence state takes the form

$$c_{coex} = \frac{4N(0)}{T_s^2}\int_0^W d\varepsilon \left(\frac{e^{\sqrt{\varepsilon^2+\Delta_c^2}/T_s}}{\left(e^{\sqrt{\varepsilon^2+\Delta_c^2}/T_s}+1\right)^2}\left(2\varepsilon^2+2\Delta_c^2-T_s\left(\frac{d\Delta_s^2}{dT}+\frac{d\Delta_c^2}{dT}\right)_{coex}\right)\right), \tag{3.86}$$

where the derivative of gap at T_s can be determined from eq.(3.64) and (3.65). Differentiating them with respect to T at near T_s, then taking the limit $T \to T_s$, we get the system of equations

$$0.5 + X1 = \frac{1}{T}\frac{d\Delta_c^2}{dT}X2 + \frac{1}{T}\frac{d\Delta_s^2}{dT}X3\,,$$
$$0.5 + X4 = \frac{1}{T}\frac{d\Delta_c^2}{dT}X5 + \frac{1}{T}\frac{d\Delta_s^2}{dT}X6\,,$$

where

$$X1 = \sum_{m=1} B_m\, 2m(2m+1)r^{2m} \quad ,X2 = \sum_{m=1}\frac{B_m}{\pi^2}m(2m+1)r^{2m-2},$$
$$X3 = \sum_{m=1}\frac{B_m}{\pi^2}\frac{m(2m+1)(2m-1)}{3}r^{2m-2} \quad ,X4 = \sum_{m=1} B_m\, 2mr^{2m}\,, \tag{3.87}$$
$$X5 = \sum_{m=1}\frac{B_m}{\pi^2}mr^{2m-2}, r = \frac{\Delta_c}{\pi T_s}.$$

After solving the system of equation we have

$$\left(\frac{1}{T}\frac{d\Delta_c^2}{dT}\right)_{coex} = \frac{0.5X3 + X4X3 - 0.5X2 - X2X1}{X5X3 - X2X2},$$
$$\left(\frac{1}{T}\frac{d\Delta_s^2}{dT}\right)_{coex} = \frac{0.5+X1}{X3} - \frac{X2X2}{(X5X3-X2X2)}\left(\frac{0.5+X4}{X2}-\frac{0.5+X1}{X3}\right). \tag{3.88}$$

To consider the specific heat jump at T_s, we also have to consider the specific heat of pure CDW state at a given T_s

$$c_{CDW}\,(T_s) = \frac{4N(0)}{T_s^2}\int_0^W d\varepsilon \left(\frac{e^{\sqrt{\varepsilon^2+\Delta_c^2}/T_s}}{\left(e^{\sqrt{\varepsilon^2+\Delta_c^2}/T_s}+1\right)^2}\left(\varepsilon^2+\Delta_c^2-\frac{T_s}{2}\left(\frac{d\Delta_c^2}{dT}\right)_{CDW}\right)\right). \qquad (3.89)$$

Differentiating eq.(3.67), we have

$$\frac{1}{T_s}\left(\frac{d\Delta_c^2}{dT}\right)_{CDW} = \frac{0.5+X4}{X5}. \qquad (3.90)$$

At near T_c the system is pure CDW the result is same as pure SDW

$$\frac{\Delta c}{c_n} = \frac{c_{CDW}-c_n}{c_n} = \frac{12}{7\xi(3)} = 1.426\,. \qquad (3.91)$$

10.2 Specific Heat at Near Zero-Temperature

Applying the following relation to eq.(3.41)

$$2\mathrm{Cosh}\left(\frac{\sqrt{\varepsilon_k^2+\Delta_\pm^2}}{2T}\right) = e^{E^\pm/2T}+e^{-E^\pm/2T} = e^{E^\pm/2T}\left(1+e^{-E^\pm/T}\right)$$

, at near zero temperature the free energy becomes

$$\Omega = \frac{\Delta_s^2}{V^s}+\frac{\Delta_c^2}{V^c}-N(0)\left(2W^2+\frac{\Delta_+^2}{2}+\frac{\Delta_-^2}{2}+\Delta_+^2\mathrm{Log}\left[\frac{2W}{|\Delta_+|}\right]+\Delta_-^2\mathrm{Log}\left[\frac{2W}{|\Delta_-|}\right]\right)$$
$$-2N(0)\int_0^W d\varepsilon\left(2Te^{-\frac{\sqrt{\varepsilon^2+\Delta_+^2}}{T}}+2Te^{-\frac{\sqrt{\varepsilon^2+\Delta_-^2}}{T}}\right) \qquad (3.92)$$

From the zero gap equation the first two terms can be expressed as

$$\frac{\Delta_s^2}{V^s}+\frac{\Delta_c^2}{V^c} = N(0)\left(\frac{\Delta_s^2\Delta_+(0)}{\Delta_s(0)}\ln\left[\frac{2W}{|\Delta_+(0)|}\right]+\frac{\Delta_s^2\Delta_-(0)}{\Delta_s(0)}\ln\left[\frac{2W}{|\Delta_-(0)|}\right]\right)$$
$$+N(0)\left(\frac{\Delta_c^2\Delta_+(0)}{\Delta_c(0)}\ln\left[\frac{2W}{|\Delta_+(0)|}\right]-\frac{\Delta_c^2\Delta_-(0)}{\Delta_c(0)}\ln\left[\frac{2W}{|\Delta_-(0)|}\right]\right)$$
$$\approx N(0)\left(\Delta_+\Delta_+(0)\ln\left[\frac{2W}{|\Delta_+(0)|}\right]+\Delta_-\Delta_-(0)\ln\left[\frac{2W}{|\Delta_-(0)|}\right]\right)$$

Substituting this approximation in eq.(3.92), we have

$$\Omega \approx -\mathrm{N}(0)(2\mathrm{W}^2 + \Delta_s^2(0) + \Delta_c^2(0)) \\ - 4\mathrm{TN}(0)\int_0^{\mathrm{W}} d\varepsilon \left(e^{-\frac{\sqrt{\varepsilon^2+\Delta_+^2(0)}}{\mathrm{T}}} + e^{-\frac{\sqrt{\varepsilon^2+\Delta_-^2(0)}}{\mathrm{T}}} \right).$$

The integral can be represented by the Bessel function

$$\int_0^{\mathrm{W}} d\varepsilon\, e^{-\frac{\sqrt{\varepsilon^2+\Delta_+^2(0)}}{\mathrm{T}}} = \Delta_+ \int_1^{\infty} \frac{y e^{-\frac{\Delta_+}{\mathrm{T}}y}}{\sqrt{y^2-1}} dy = \Delta_+ \mathrm{K}_1\left(\frac{\Delta_+}{\mathrm{T}}\right).$$

Then we get

$$\Omega \approx -\mathrm{N}(0)(2\mathrm{W}^2 + \Delta_s^2(0) + \Delta_c^2(0)) \\ - 4\mathrm{TN}(0)\left(\Delta_+ \mathrm{K}_1\left(\frac{\Delta_+}{\mathrm{T}}\right) + |\Delta_-| \mathrm{K}_1\left(\frac{|\Delta_-|}{\mathrm{T}}\right) \right). \tag{3.93}$$

The last term can be calculated using the same technique as in the section of the near zero temperature gap. Therefore, the free energy at near zero temperature is approximately given by

$$\Omega \approx -\mathrm{N}(0)(2\mathrm{W}^2 + \Delta_s^2(0) + \Delta_c^2(0)) \\ - 2\mathrm{TN}(0)\left(e^{-\frac{\Delta_+(0)}{\mathrm{T}}} \sqrt{2\pi \mathrm{T} \Delta_+(0)} + e^{-\frac{\Delta_-(0)}{\mathrm{T}}} \sqrt{2\pi \mathrm{T} \Delta_-(0)} \right). \tag{3.94}$$

From this we have

$$\mathrm{S} = -\frac{\partial \Omega}{\partial \mathrm{T}} \approx 2\mathrm{N}(0)\left(\left(\Delta_+(0)\right)^{\frac{3}{2}} e^{-\frac{\Delta_+(0)}{\mathrm{T}}} \sqrt{\frac{2\pi}{\mathrm{T}}} + \left(\Delta_-(0)\right)^{\frac{3}{2}} e^{-\frac{\Delta_-(0)}{\mathrm{T}}} \sqrt{\frac{2\pi}{\mathrm{T}}} \right), \tag{3.95}$$

$$\mathrm{C} = \mathrm{T}\frac{\partial \mathrm{S}}{\partial \mathrm{T}} \approx 2\mathrm{N}(0)\sqrt{\frac{2\pi}{\mathrm{T}^3}}\left(\left(\Delta_+(0)\right)^{\frac{5}{2}} e^{-\frac{\Delta_+(0)}{\mathrm{T}}} + \left(\Delta_-(0)\right)^{\frac{5}{2}} e^{-\frac{|\Delta_-|(0)}{\mathrm{T}}} \right). \tag{3.96}$$

CHAPTER 4
RESULTS AND DISCUSSIONS

In this chapter the results of the calculation in chapter 3 will be discussed. Before going into detailed discussion, in order to introduce the general feature of the interplay of the SDW and CWD we will briefly present some of the results of the solving self-consistence gap equation numerically. From eq.(3.28) and (3.29) we have by converting summation to integration with the constant DOS N(0)

$$\Delta_s = g_s \int_0^W d\varepsilon \left\{ \frac{\Delta_+}{\sqrt{\varepsilon^2+\Delta_+^2}} \mathrm{Tanh}\left(\frac{\sqrt{\varepsilon^2+\Delta_+^2}}{2T}\right) + \frac{\Delta_-}{\sqrt{\varepsilon_k^2+\Delta_-^2}} \mathrm{Tanh}\left(\frac{\sqrt{\varepsilon^2+\Delta_-^2}}{2T}\right) \right\},$$

$$\Delta_c = g_c \int_0^W d\varepsilon \left\{ \frac{\Delta_+}{\sqrt{\varepsilon^2+\Delta_+^2}} \mathrm{Tanh}\left(\frac{\sqrt{\varepsilon^2+\Delta_+^2}}{2T}\right) - \frac{\Delta_-}{\sqrt{\varepsilon^2+\Delta_-^2}} \mathrm{Tanh}\left(\frac{\sqrt{\varepsilon^2+\Delta_-^2}}{2T}\right) \right\}$$

where $g_s = V^s N(0)$, $g_c = V^c N(0)$, $\Delta_\pm = \Delta_s \pm \Delta_c$ and $W = 4t_o$. To perform the numerical integration introducing the dimensionless quantity $x = \varepsilon/t_o, z_{s,c} = \Delta_{s,c}/t_o, t = T/t_o$ we have

$$z_s = g_s \int_0^4 dx \left\{ \frac{z_+}{\sqrt{x^2+z_+^2}} \mathrm{Tanh}\left(\frac{\sqrt{x^2+z_+^2}}{2t}\right) + \frac{z_-}{\sqrt{x^2+z_-^2}} \mathrm{Tanh}\left(\frac{\sqrt{x^2+z_-^2}}{2t}\right) \right\},$$

$$z_c = g_c \int_0^4 dx \left\{ \frac{z_+}{\sqrt{\varepsilon^2+z_+^2}} \mathrm{Tanh}\left(\frac{\sqrt{x^2+z_+^2}}{2t}\right) - \frac{z_-}{\sqrt{\varepsilon^2+\Delta_-^2}} \mathrm{Tanh}\left(\frac{\sqrt{x^2+z_-^2}}{2t}\right) \right\}.$$

The results of the numerical calculation for $g_c = 0.0760$, $g_s = 0.0850$ are shown in figure 19. The dashed lines represent the pure SDW and CDW gaps. The zero temperature gap and critical temperature of the pure state agree well with the BCS value of $2\Delta_{so,co}/T_{so,co}$. Here Δ_{so}, Δ_{co} ,T_{so} and T_{co} denote zero temperature gap and critical temperature for pure SDW and CDW, respectively.

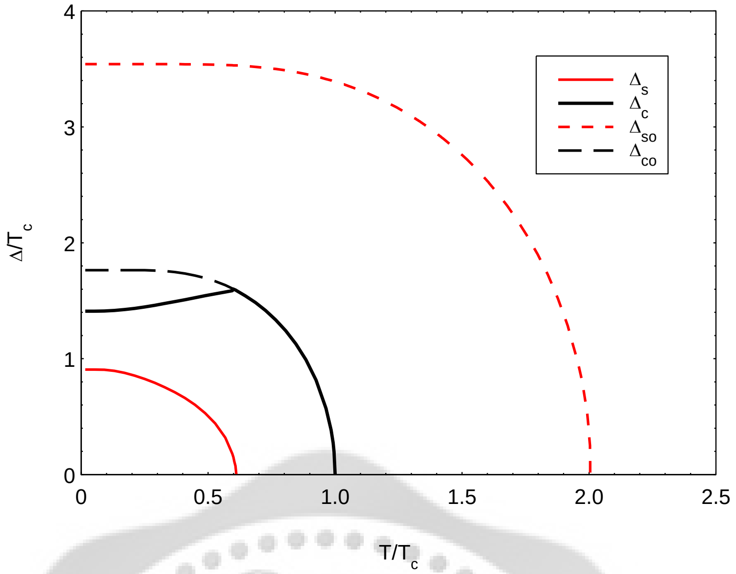


Figure 19 Temperature dependence of gap from numerical calculation for g_c = 0.0760, g_s = 0.0850

For the coexistence state the CDW gap opens up at higher temperature T_c (t_c=0.00630) and grows with the lowering temperature. Its growth is arrested at T_s (t_s=0.00385) due to the onset of SDW. It is suppressed below T = T_s while SDW gap is suppressed for all temperature range. Their zero temperature gaps are smaller compared to that of pure states. The importance effect of the interplay between SDW and CDW is to suppress the SDW critical temperature T_s, but there is no effect on the CDW critical temperature T_c. From the figure 19 we have

$$\frac{T_s}{T_c} = 0.611, \quad \frac{T_{so}}{T_c} = 2, \quad \frac{2\Delta_s(0)}{T_s} = 2.97, \frac{2\Delta_c(0)}{T_c} = 2.82\,.$$

Their gap-to-T_c ratios are lighter than that of BCS value of 3.53. In the subsequent sections we will try to find out the expression of the gaps and critical temperature as well as their related quantities approximately.

1 Zero-Temperature Gaps

From eq.(3.55) and (3.56) , the zero temperature gap are

$$\Delta_s(0) = 2We^{-\frac{1}{2g_s}}f(1/a) = \Delta_{so}(0)f(1/a), \tag{4.1}$$

$$\Delta_c(0) = 2We^{-\frac{1}{2g_c}}f(a) = \Delta_{co}(0)f(a) \tag{4.2}$$

,where

$$a = \frac{\Delta_s(0)}{\Delta_c(0)}, f(a) = \frac{1}{\sqrt{|1-a|^{1-a}|a+1|^{1+a}}}.$$

Our Formula of zero temperature gaps are rather similar to the previous study of the coexistence of SDW and superconductivity by S.N. Behera and S. Bhattacharya**(**Beher; & Bhattacharya. 1990: 112-126**).**The dependence of f(1/a) and f(a) on the ratio a are shown in figure 20. It indicates that for the coexistence state, due to the interplay between SDW and CDW, the zero temperature gaps do not exceed that of pure state; $\Delta_s(0) \leq \Delta_{so}(0)$, $\Delta_c(0) \leq \Delta_{co}(0)$,.

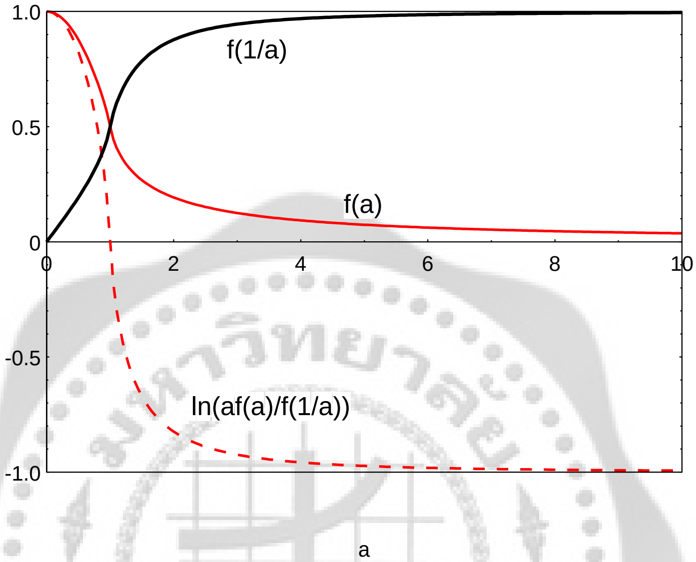


Figure 20 the dependence of f(1/a), f(a) and ln(af(1/a)/f(a)) on the ratio a.

In the limit of $a \to \infty$ correspond to pure SDW; $\Delta_s(0) = \Delta_{so}(0) = 2We^{-1/2g_s}$; $\Delta_c(0) = 0$. . And in the limit of $a \to 0$ corresponds to pure CDW state; $\Delta_c(0) = \Delta_{co}(0) = 2We^{-1/2g_c}$; $\Delta_s(0) = 0$.To calculate the zero temperature gap from the given values of g_s and g_c, dividing eq.(4.2) by eq.(4.1), and taking logarithm , we have

$$\ln\left(a\frac{f(a)}{f(1/a)}\right) = \frac{1}{2}\left(\frac{1}{g_c} - \frac{1}{g_s}\right). \qquad 4.3$$

This equation and the plot of the left hand side of eq.(4.3) shown in figure 20 give us the condition; $\Delta_s(0) < \Delta_c(0)$ if $g_s > g_c(\Delta_{so}(0) > \Delta_{co}(0))$ and $\Delta_s(0) > \Delta_c(0)$ if $g_s < g_c$.The SDW and CDW zero temperature gap can be easily calculated by inserting the ratio a solving from eq.(4.3) to eq.(4.1) and eq.(4. 2).

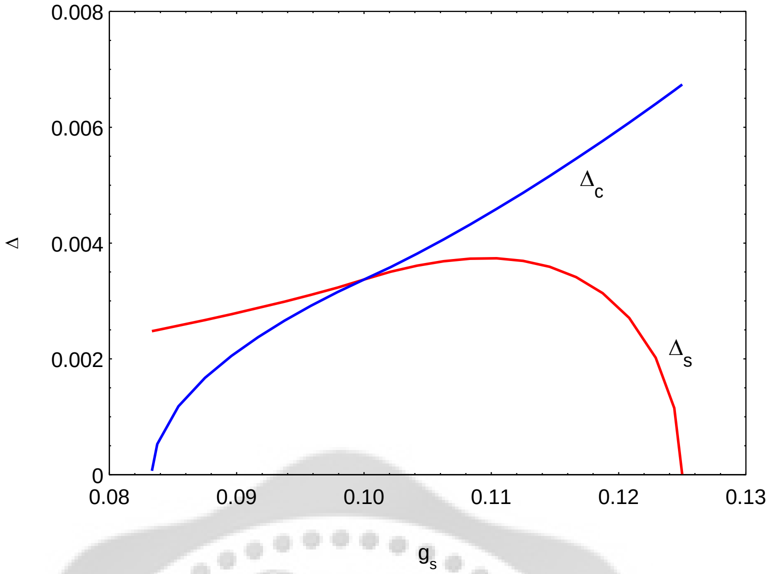


Figure 21 Effective potential dependence of the SDW and CDW gap for g_c=0.085.

Figure 21 shows the dependence of SDW and CDW gap on the coupling constant g_s. All expression of energy quantity is in the unit of t_o. Both states coexist from g_s = 0.083 to 0.125. To obtain the phase diagram we consider the left hand side of eq.(4.3) as shown in figure 20. It takes the value in the range of (-1,1). Therefore, we get the condition of coexist of SDW and CDW as

$$-2 < 1/g_c - 1/g_s < 2\,. \tag{4.4}$$

This equation gives us the equation of phase boundary. The phase diagram of SDW and CDW states at zero temperature in coupling constant plane are shown in figure 22.

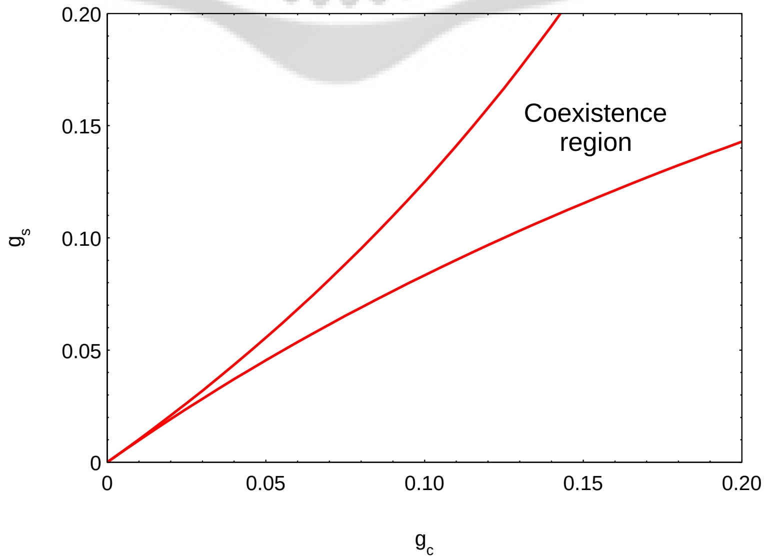


Figure 22 Phase diagram of SDW and CDW state in coupling constant plane.

The coexistence region is a region along a diagonal line $g_s = g_c$. Its width increases with increase in coupling constants. Outside the coexistence region there should be a single stable phase depends on the strength of the interaction, i.e., if the electron-phonon attractive interaction (V^c or g_c) is stronger than the Coulomb repulsive interaction between electrons (V^s or g_s) and they violate eq.(4.4) the stable state would be the CDW state and vice versa. Furthermore in figure 22 it is clearly seen that the SDW and CDW states are symmetric in the phase diagram because their gap equations are symmetric (eqs.(3.28) and (3.29)).

2 Critical Temperature

2.1 Case 1.T_c>T_s The SDW critical temperature T_s is given by eq.(3.69)

$$T_s = \frac{2\gamma W}{\pi} \mathrm{Exp}\left\{ -\frac{1}{2}\left(\frac{1}{2g_c} + \frac{1}{2g_s}\right) + 2\sum_{m=1} B_m \,(m+1)\left(\frac{\Delta_c}{\pi T_s}\right)^{2m} \right\} \tag{4.5}$$

,where $\Delta_c/\pi T_s$ can be evaluated from

$$\left(\frac{1}{2g_c} - \frac{1}{2g_s}\right) = -4\sum_{m=1} B_m \, m \left(\frac{\Delta_c}{\pi T_s}\right)^{2m}. \tag{4.6}$$

The series on the right side is converge if $\Delta_c/\pi T_s < 1$ as we assumed before in section 3.7. Here and further on our calculation will be limited by the condition $0 < \Delta_c/\pi T_s < 1$ .The right hand side of eq.(4.6) is positive definite, this means that the condition for $T_c > T_s$ if and only if $g_s > g_c$ and vice versa for $T_s > T_c$. To calculate the value of T_s from the given value of g_s and g_c, we can simplify eq.(4.5) and (4.6) by replacing them by a best fitted curves. The series in eq.(4.5) and (4.6) can be represented by 4th order polynomials

$$\sum_{m=1} B_m \,(m+1)\left(\frac{\Delta_c}{\pi T_s}\right)^{2m} = 0.029r - 1.366r^2 + 1.089r^3 - 0.269r^4, \tag{4.7}$$

$$\textstyle\sum_{m=1} B_m \, m \left(\frac{\Delta_c}{\pi T_s}\right)^{2m} = 0.0183r - 0.728r^2 + 0.726r^3 - 0.216r^4. \tag{4.8}$$

Figure 23 demonstrates the comparison between the fitted curve and the series of eqs.(4.7) and (4.8).

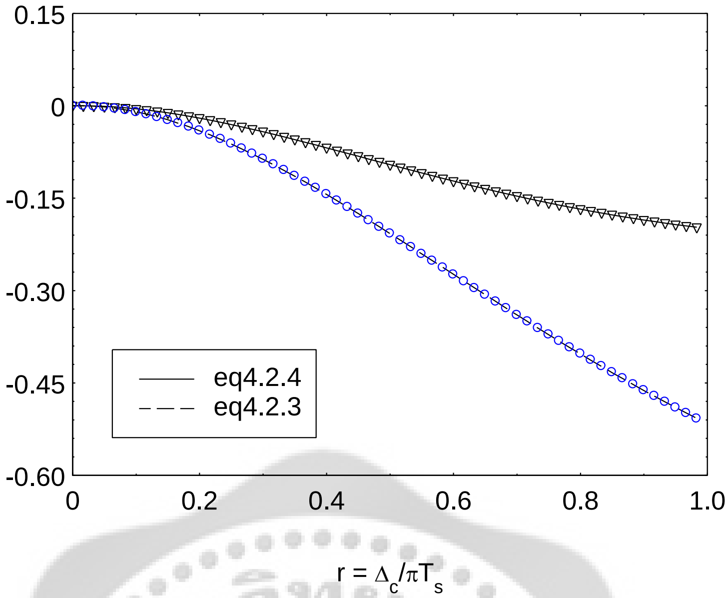


Figure 23 the comparison between the fitted curve and the series of eq.(4.7) and (4.8).

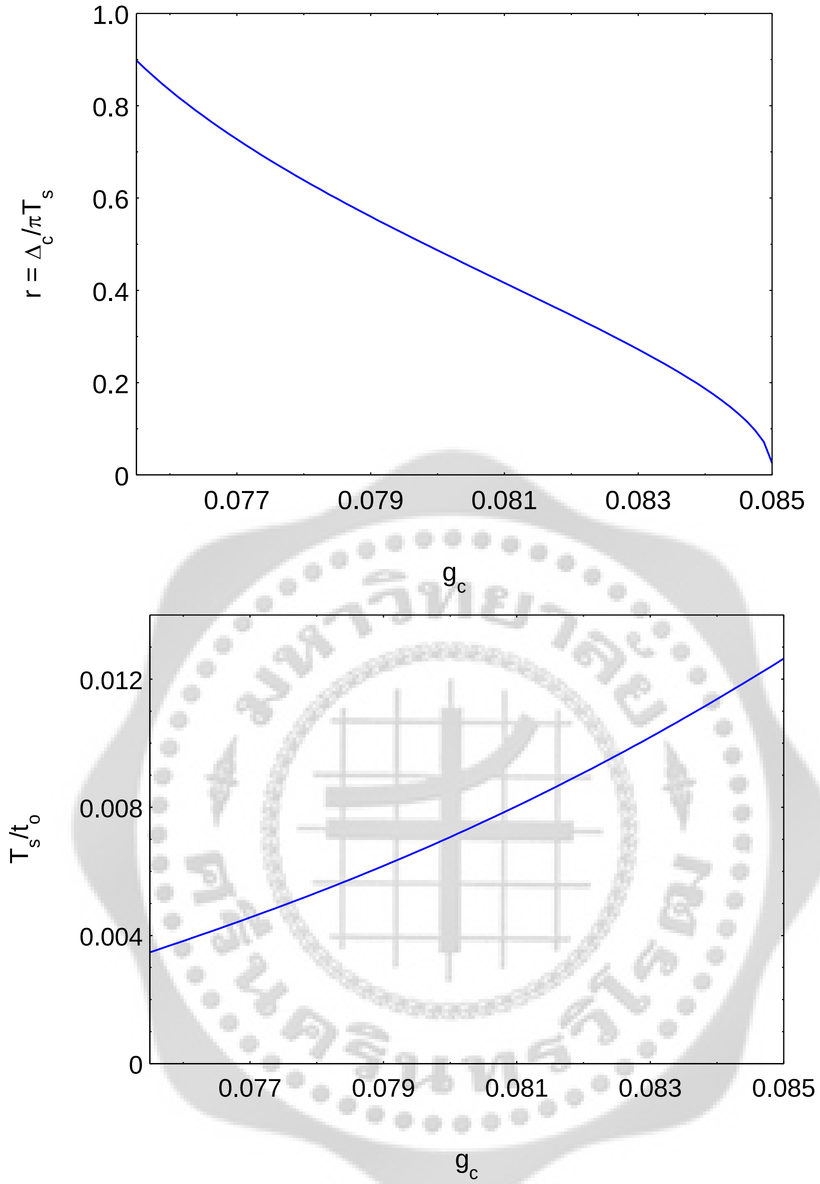
Then the T_s can be written as

$$T_s = \frac{2\gamma W}{\pi} \mathrm{Exp}\left(-\frac{1}{2}\left(\frac{1}{2g_c} + \frac{1}{2g_s}\right) + 2(0.029r - 1.366r^2 + 1.089r^3 - 0.2689r^4) \right) \quad (4.9)$$

,where the parameter r = $\Delta_c/\pi T_s$ is a positive real root of the following equation

$$\left(\frac{1}{2g_c} - \frac{1}{2g_s}\right) = -4(0.0183r - 0.728r^2 + 0.726r^3 - 0.216r^4)\,. \quad (4.10)$$

Figure 24 shows the dependence of r and T_s/t_o on g_c for g_s = 0.085 calculated from eqs.(4.9) and (4.10). The parameter r gradually decrease with increase in g_c and becomes zero at g_c= g_s. The parameter r = 0 or Δ_c = 0 atT_s implies that T_s =T_c. T_s/t_o increases with increase in g_c. This indicates that the interaction responding to CDW state can enhance the SDW critical temperature T_s. Due to the symmetry we can expect that the plot of r = $\Delta_s/\pi T_c$ and T_c/t_o against g_s are similar to figure 24.



(a)

(b)

Figure 24 The dependence of r (a) and T_s/t_o (b) on g_c for fixed $g_s = 0.085$.

At T_c eq.(3.70) gives

$$T_c = \frac{2\gamma W}{\pi} e^{-1/2g_c} = T_{co}\ . \tag{4.11}$$

This shows that the interplay has no effect on CDW critical temperature T_c if $g_s > g_c$.

T_s in eq.(4.5) can be also written as

$$T_s = \frac{2\gamma W}{\pi} e^{-\frac{1}{2g_s}} \mathrm{Exp}\left(-\frac{1}{2}\left(\frac{1}{2g_c} - \frac{1}{2g_s}\right) + 2\sum_{m=1} B_m\,(m+1)\left(\frac{\Delta_c}{\pi T_s}\right)^{2m}\right).$$

From eq.(4.6) and $T_{so} = (2\gamma W/\pi)e^{-1/2gs}$, we have

$$T_s = T_{so}\,\mathrm{Exp}\left(2\sum_{m=1} B_m\,(2m+1)\left(\frac{\Delta_c}{\pi T_s}\right)^{2m}\right). \tag{4.12}$$

The series in the parenthesis is negative definite. This means that $T_s \le T_{so}$. Hence, we can conclude that for $g_s > g_c$ the interplay between SDW and CDW suppress the SDW critical temperature.

T_s in eq.(4.5) can be also rewritten in term of the CDW critical temperature as

$$T_s = \frac{2\gamma W}{\pi} e^{-1/2g_c}\,\mathrm{Exp}\left(\frac{1}{2}\left(\frac{1}{2g_c} - \frac{1}{2g_s}\right) + 2\sum_{m=1} B_m\,(m+1)\left(\frac{\Delta_c}{\pi T_s}\right)^{2m}\right).$$

Using 4.6 and 4.11, we get

$$T_s = T_c\,\mathrm{Exp}\left(2\sum_{m=1} B_m\left(\frac{\Delta_c}{\pi T_s}\right)^{2m}\right). \tag{4.13}$$

We also have

$$\frac{T_{so}}{T_c} = \mathrm{Exp}\left(\frac{1}{2g_c} - \frac{1}{2g_s}\right) = \mathrm{Exp}\left(-4\sum_{m=1} B_m\, m\left(\frac{\Delta_c}{\pi T_s}\right)^{2m}\right). \tag{4.14}$$

Using $\Delta_c/\pi T_s$ as a parameter, eq.(4.13) and (4.14) enable us to plot the temperature phase diagram as shown in figure 25. In the figure the vertical axis is a reduced temperature T/T_c and a horizontal axis is T_{so}/T_c which is related to the coupling constant via $\ln(T_{so}/T_c)=(g_s-g_c)/2g_sg_c$. There are two regions of coexistence and pure CDW state separated by the phase boundary line. The phase transition takes place from CDW to coexistence state when the system crosses this line by lowering temperature. This transition temperature or SDW critical temperature decreases with the increase in T_{so}/T_c. In the other word the SDW critical temperature decreases with the increase in g_s or the decrease in g_c. While the transition from normal state to CDW state occur at $T = T_c$.

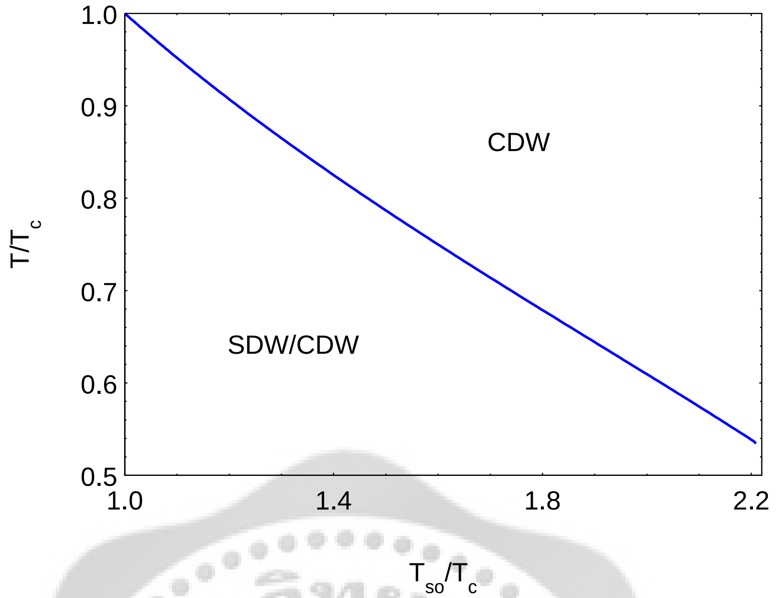
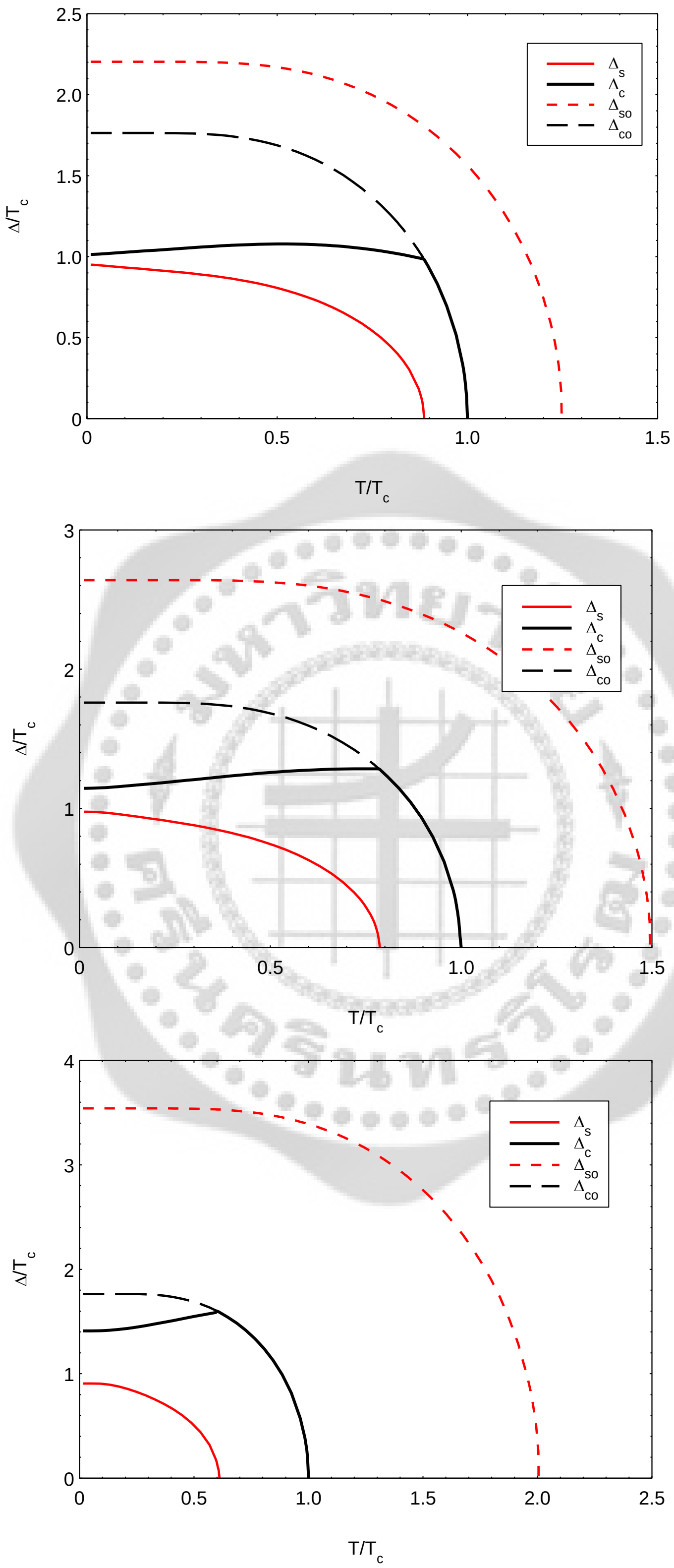


Figure 25 Phase diagram of SDW and CDW state temperature plane.

Figure 26 shows the temperature dependence of SDW and CDW gaps for T_{so}/T_c=1.25, 1.5 and 2 from numerical solving of self-consistence equations. They agree well with Fig.4.7 with the reduced transition temperature from CDW to coexistence state of ~0.9, 0.8 and 0.6, respectively. Furthermore, figure 26 shows that $\Delta/\pi T_s$ <1 satisfies our approximation assumption.



(a)

(b)

(c)

Figure 26 the temperature dependence of gap for (a) T_{so}/T_c =1.25, (b) T_{so}/T_c =1.5, (c) T_{so}/T_c =2, dashed line for pure states.

2.2 Case 2. $T_s > T_c$ Due to the symmetry of gap equations, for this case we can expect the following relations

$$\left(\frac{1}{2g_s}-\frac{1}{2g_c}\right) = -4\sum_{m=1} B_m\, m \left(\frac{\Delta_s}{\pi T_c}\right)^{2m}, \tag{4.15}$$

$$T_c = \frac{2\gamma W}{\pi}\mathrm{Exp}\left(-\frac{1}{2}\left(\frac{1}{2g_c}+\frac{1}{2g_s}\right)+2\sum_{m=1} B_m\,(m+1)\left(\frac{\Delta_s}{\pi T_c}\right)^{2m}\right), \tag{4.16}$$

$$T_s = \frac{2\gamma W}{\pi}e^{-1/2g_s} = T_{so}, \tag{4.17}$$

$$T_c = T_s \mathrm{Exp}\left(2\sum_{m=1} B_m \left(\frac{\Delta_s}{\pi T_c}\right)^{2m}\right), \tag{4.18}$$

$$\frac{T_{co}}{T_s} = \mathrm{Exp}\left(\frac{1}{2g_s}-\frac{1}{2g_c}\right) = \mathrm{Exp}\left(-4\sum_{m=1} B_m\, m\left(\frac{\Delta_s}{\pi T_c}\right)^{2m}\right), \tag{4.19}$$

$$T_c = T_{co}\,\mathrm{Exp}\left(2\sum_{m=1} B_m\,(2m+1)\left(\frac{\Delta_s}{\pi T_c}\right)^{2m}\right). \tag{4.20}$$

These are identical to the case.1 by interchanging indices s and c. Eq.(4.15) reveals that $T_c < T_s$ if $g_c > g_s$. And eq.(4.20) implies that $T_c \leq T_{co}$. From eqs.(4.18) and (4.19) we obtain the temperature phase diagram similar to that of figure 25.

This section can be summarized that interplay between SDW and CDW leads to the competition not the enhancement with the following feathers;

1. For $g_s > g_c$ ($T_{so} > T_{co}$) the interplay between SDW and CDW has no effect on CDW critical temperature; $T_c = T_{co}$ while it suppress SDW critical temperature $T_s < T_{so}$ and $T_s < T_c$.

2. For $g_c > g_s$ ($T_{co} > T_{so}$) SDW critical temperature is unchanged by the competition between SDW and CDW;$T_s = T_{so}$,but CDW critical temperature is suppressed; $T_c < T_{co}$ and $T_c < T_s$.

3. In the case of $g_c = g_s$we have $T_s = T_{so}= T_{co}= T_c$.

It should be noted that our results of T_s and T_c are in contrast to the previous study by Pradhan et at(Pradhan; et al. 2008: 2332-2335). They have solved the self-consistence equations and shown that the interplay between SDW and CDW leads to the enhancement of the CDW critical temperature for $g_s > g_c$. While in our study if $g_s > g_c$ T_c is unchanged; T_c=T_{co}.

3 The Gap-to-T_c Ratio

Without loss of generality, here and further on we assume that $T_c > T_s$. Using eqs.(4.1), (4.2),(4.11) and (4.12), we get the zero gap to critical temperature ratio at T_s and T_c as follow

$$\frac{2\Delta_s(0)}{T_s} = \frac{2\pi}{\gamma} f(1/a)\mathrm{Exp}\left(-2\sum_{m=1} B_m\,(2m+1)\left(\frac{\Delta_c}{\pi T_s}\right)^{2m}\right) \tag{4.21}$$

$$\frac{2\Delta_c(0)}{T_c} = \frac{2\pi}{\gamma} f(a) \tag{4.22}$$

It follows from eq.(4.3) and (4.6) that we have

$$\ln\left(a\frac{f(a)}{f(1/a)}\right) = -4\sum_{m=1} B_m\, m\left(\frac{\Delta_c}{\pi T_s}\right)^{2m} \tag{4.23}$$

, which can be used to evaluated the ratio a. Figure 27 demonstrates the variation of the gap-to-T_c ratio as a function of T_{so}/T_c.

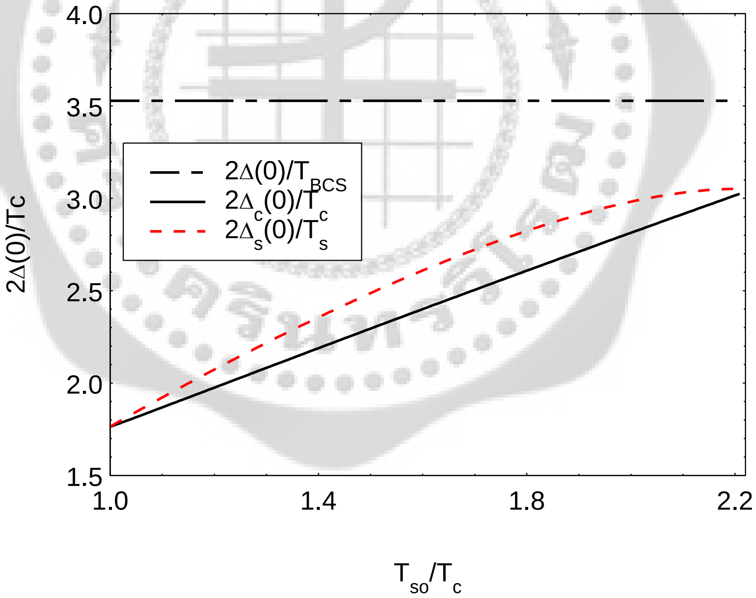


Figure 27 gap-to-T_c ratio as a function of T_{so}/T_c.

It is clearly seen that for the coexistence states $2\Delta_c(0)/T_c$ and $2\Delta_s(0)/T_s$ are depend on their critical temperature and their value are less than the typical BCS value of 3.52. However, it will be seen in the next section that the observable gap would be the effective gaps Δ_+ and Δ_- instead. The zero temperature effective gap to critical temperature are given by

$$\frac{2\Delta_{\pm}(0)}{T_s} = \frac{2\pi}{\gamma} f\left(\frac{1}{a}\right) \mathrm{Exp}\left(-2\sum_{m=1} B_m\,(2m+1)\left(\frac{\Delta_c}{\pi T_s}\right)^{2m}\right)$$
$$\pm\frac{2\pi}{\gamma} f(a)\mathrm{Exp}\left(-2\sum_{m=1} B_m\left(\frac{\Delta_c}{\pi T_s}\right)^{2m}\right), \tag{4.24}$$
$$\frac{2\Delta_{\pm}(0)}{T_c} = \frac{2\pi}{\gamma} f\left(\frac{1}{a}\right) \mathrm{Exp}\left(-4\sum_{m=1} B_m\, m\left(\frac{\Delta_c}{\pi T_s}\right)^{2m}\right) \pm \frac{2\pi}{\gamma} f(a).$$

Their dependence on T_{so}/T_c is shown in figure 28. Apparently, our calculation shows that the $2\Delta_+(0)/T_{s,c}$ is greater than or equal to the BCS value of 3.53 while $2\Delta_-(0)/T_{s,c}$ is smaller.

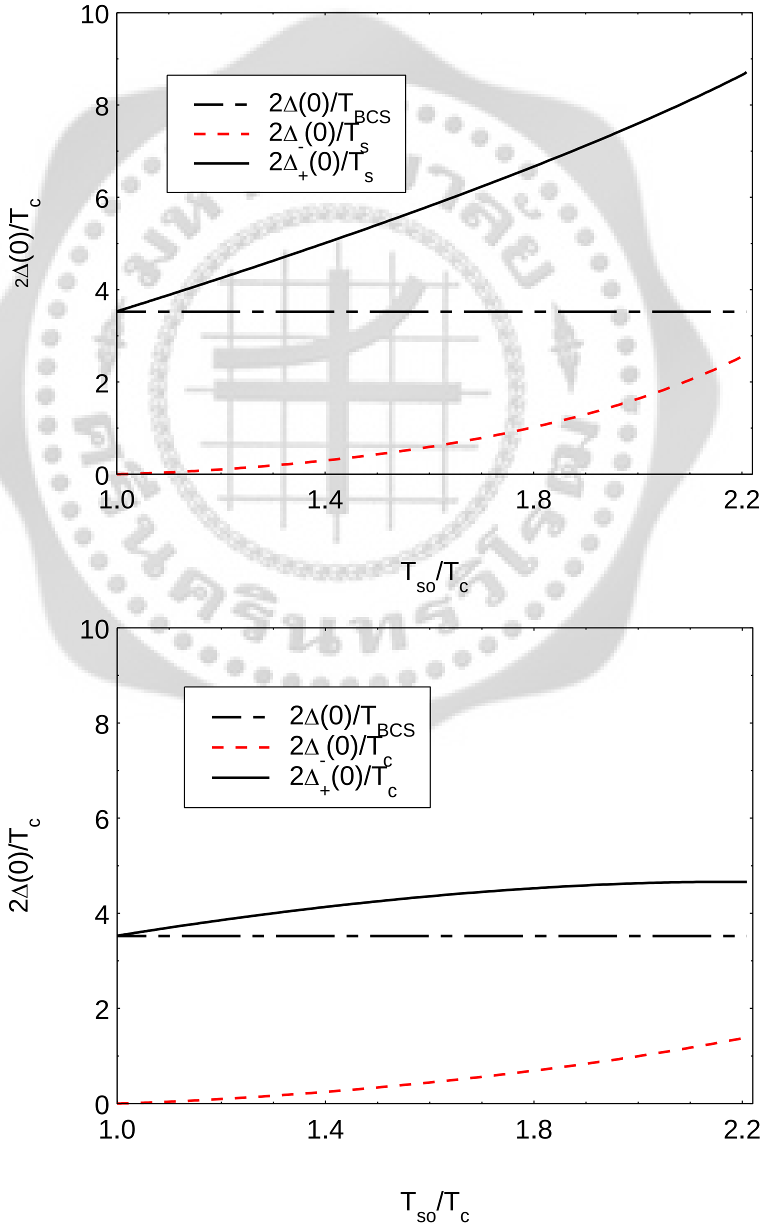


Figure 28 gap-to-T_c ratios as a function of T_{so}/T_c.

Our calculation support the gap-to-T_c ratio $2\Delta(0)/T_c$ for some type of HTS superconductor. Many experiments have shown that $2\Delta(0)/T_c$ of the HTS superconductor varies from material to material and differs from 3.53. For instance the ratio $2\Delta(0)/T_c$ is 3.8 for $Nd_{2-x}Ce_xCuO_4$**,** 3.7–3.8 for $Ba_{1-x}K_xBiO_3$ and 6.7 for heavy fermion superconductor UBe_{13}.(Bennemann; & Ketterson. 2008: 862, Buckel; & Kleiner. 2004: 165)**.**In iron based superconductor $Ba(Fe_{1-x}Co_x)_2As_2$ their ratio $2\Delta(0)/T_c$ can be explained by the two-gap model with the ratio of ~5 and ~1.9 (Hardy; et al. 2010: 47008).

4 DOS and Band Structure

The density of states is the important physical function of the system which can be measured by various techniques such as the scanning tunneling microscope (STM) or the angle resolved photoemission spectroscopy (ARPS). The DOS of the coexistence of SDW and CDW calculated from the spectral function is

$$\rho(\omega) = 2N(0)\left(\frac{|\omega|}{\sqrt{\omega^2-\Delta_+^2}}\theta(-\omega)\theta(|\omega|-\Delta_+) + \frac{|\omega|}{\sqrt{\omega^2-\Delta_-^2}}\theta(-\omega)\theta(|\omega|-\Delta_-)\right) \tag{4.25}$$

Figure 29 shows the DOS of T_{so}/T_c = 1.25 for $t=T/t_o$ = 0.004, 0.008, 0.009. For T_{so}/T_c = 1.25 the SDW critical temperature is $t=T_s/t_o$= 0.0089. Above this temperature there is a single gap of pure CDW. Below T_s the system act as the two gaps system with two effective gaps; an outer and an inner gap corresponding to Δ_+ and Δ_-, respectively. Their gap edges move to that of the CDW with increase in temperature and they merge together to be CDW at T_s. Certainly, after that CDW gap gradually decreases and finally disappear at T_c.

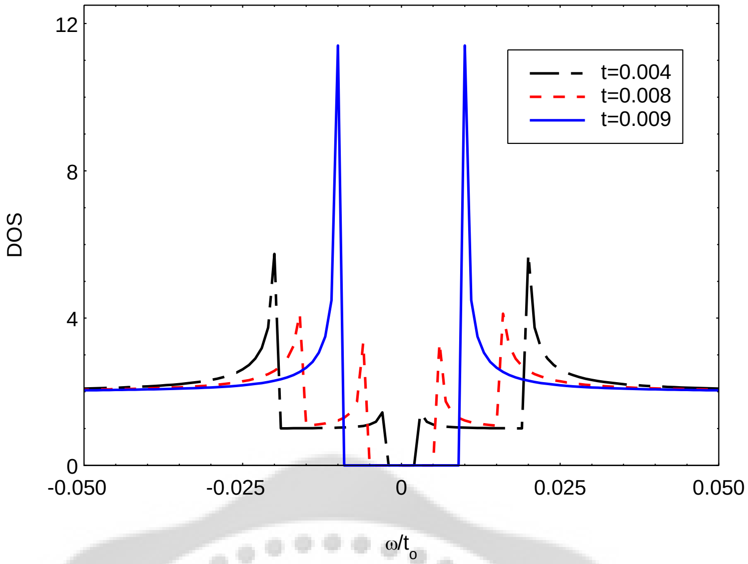


Figure 29 DOS at t=0.004,0.008 and 0.009 for T_{so}/T_c=1.25.

Figure 30 shows the Band structure (or energy dispersion) at t=0.004for T_{so}/T_c=1.25. The inset shows the energy gap at around Fermi surface (X-S line in figure 18). The presence of the energy gap around the Fermi surface leads to the lowering the energy of the system and causes the coexistence state is more stable than the normal state without gap.

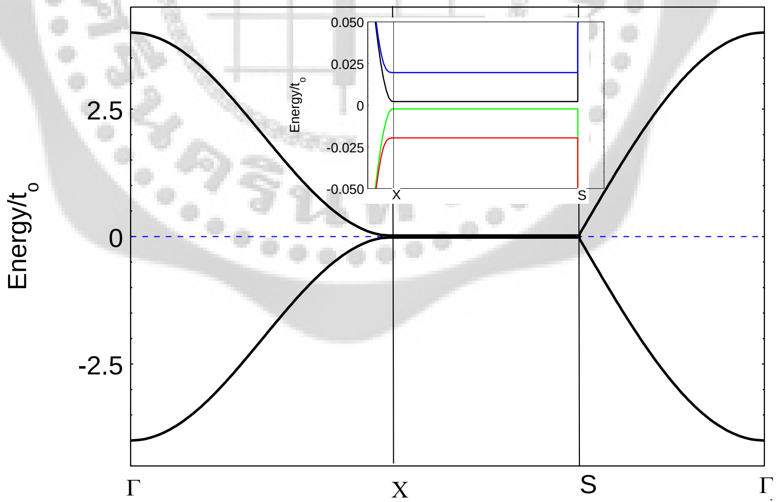


Figure 30 Band structure or dispersion curve at t=0.004for T_{so}/T_c=1.25.

5 Near Zero-Temperature and Near Critical Temperature Gaps

5.1 Near Zero-Temperature Gaps

The near zero-temperature gap for $T_c > T_s$ are given by eq.(3.80) as

$$\Delta_s(T) = \Delta_s(0) - \frac{1}{2}\left(e^{-\frac{\Delta_+(T)}{T}}\sqrt{2T\pi\Delta_+(0)} + e^{-\frac{|\Delta_-(T)|}{T}}\sqrt{2T\pi|\Delta_-(0)|}\right),$$
$$\Delta_c(T) = \Delta_c(0) - \frac{1}{2}\left(e^{-\frac{\Delta_+(T)}{T}}\sqrt{2T\pi\Delta_+(0)} - e^{-\frac{|\Delta_-(T)|}{T}}\sqrt{2T\pi|\Delta_-(0)|}\right). \qquad (4.26)$$

Since Δ_+ (T) increase while Δ_- (T) decrease with the lowering of the temperature, so that Δ_s (T) rises to Δ_s (0) while Δ_c (T) falls to Δ_c (0) . These can be clearly seen from figure 26.

5.2 Near Critical Temperature Gaps

As we assume before $T_c > T_s$, at T_s the near critical temperature gap is

$$\Delta_s^2 = \frac{8\pi^2}{7\xi(3)}\frac{T_s(T_s - T)}{(2 - X)} \qquad (4.27)$$

Where

$$X = \frac{8\pi^2}{7\xi(3)}\sum_{m=2} B_m \frac{2m(2m+1)(m+1)}{3\pi^2}\left(\frac{\Delta_c}{\pi T_s}\right)^{2m-2}. \qquad (4.28)$$

Eq.(4.27) shows that the interplay between SDW and CDW causes the near critical temperature gap smaller than the BCS value with the factor 1/(2+X). Above Ts the system becomes pure CDW then at T_c the near critical temperature gap take the same form as BCS theory

$$\Delta_c^2(T) = \frac{8\pi^2}{7\xi(3)} T_c(T_c - T). \qquad (4.29)$$

6 Specific Heat

Figure 31 shows the specific heat of coexistence, pure CDW and normal states for T_{so}/T_c=1.0,1.25,1.55.For coexistence there are specific heat jump at T_s .Above T_s the system becomes CDW state with the specific heat jump at T_c.

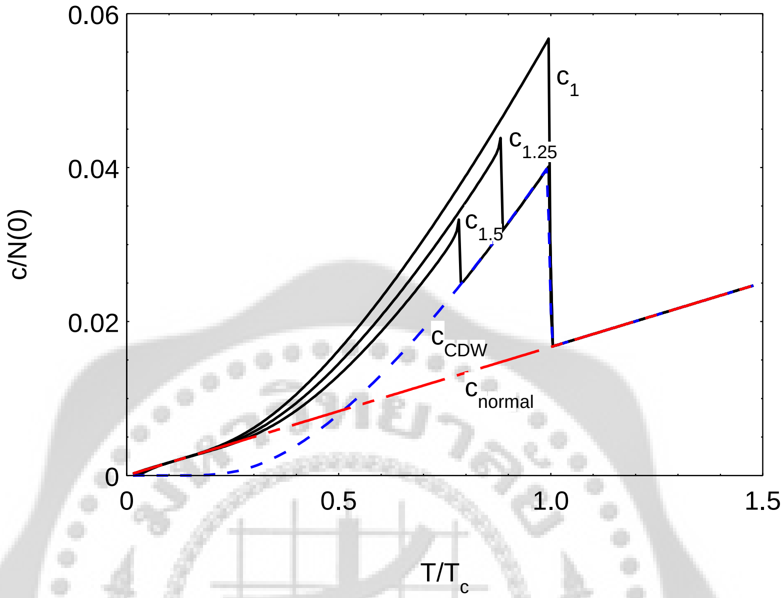


Figure 31 specific heat for T_{so}/T_c=1.55., 1.25 and 1.0

6.1 Specific Heat at Near Zero-Temperature

Near zero-temperature the specific heat is given by

$$C \approx 2N(0)\sqrt{\frac{2\pi}{T^3}}\left(\left(\Delta_+(0)\right)^{\frac{5}{2}} e^{-\frac{\Delta_+(0)}{T}} + \left(\Delta_-(0)\right)^{\frac{5}{2}} e^{-\frac{|\Delta_-(0)|}{T}}\right). \tag{4.30}$$

Figure 31 shows that for pure CDW, specific heat much smaller than normal state and it approach to zero as $e^{-\Delta c\,(0)/T}$. Unlike the case of pure CDW, for the coexistence state specific heat approach to zero as a liner function of temperature like the normal state. This would be the effect of the decreasing of $\Delta_-(0)$ in the second term in eq.(4.30). The reason behind this can be clearly seen from eq.(3.85). The gaps can be consider as constant at low temperature so we have

$$c = \frac{4N(0)}{T^2}\int_0^W d\varepsilon \left(\frac{e^{\sqrt{\varepsilon^2+\Delta_+^2}/T}}{\left(e^{\sqrt{\varepsilon^2+\Delta_+^2}/T}+1\right)^2}(\varepsilon^2+\Delta_+^2) + \frac{e^{\sqrt{\varepsilon^2+\Delta_-^2}/T}}{\left(e^{\sqrt{\varepsilon^2+\Delta_-^2}/T}+1\right)^2}(\varepsilon^2+\Delta_-^2) \right).$$

Since the $\Delta_-(0)$ decreases and rather small the last term would exhibits the normal state behavior at low temperature. While the $\Delta_+(0)$ increases and quite large compared to $\Delta_-(0)$ then the first term decreases exponentially to zero at low temperature like a pure CDW.

6.2 Specific Heat at Near Critical Temperature

From eq.(3.86) at T_s we have specific heat for the coexistence states

$$\frac{c_{coex}}{4N(0)T_s} = \int_0^{W/T_s} dx \left(\frac{e^{\sqrt{x^2+c^2}}}{\left(e^{\sqrt{x^2+c^2}}+1\right)^2} \left(2x^2 + 2c^2 - \left(\frac{1}{T_s}\frac{d\Delta_s^2}{dT} + \frac{1}{T_s}\frac{d\Delta_c^2}{dT} \right)_{coex} \right) \right) \tag{4.31}$$

,where $\varepsilon/T_s = x$; $\Delta_c/T_s = c$. The derivative of gap for coexistence state can be directly calculated from eq.(3.87) and (3.88). For pure CDW state we have

$$\frac{c_{CDW}(T_s)}{4N(0)T_s} = \int_0^{W/T_s} dx \left(\frac{e^{\sqrt{x^2+c^2}}}{\left(e^{\sqrt{x^2+c^2}}+1\right)^2} \left(x^2 + c^2 - \frac{1}{2}\left(\frac{1}{T_s}\frac{d\Delta_c^2}{dT} \right)_{CDW} \right) \right) \tag{4.32}$$

The derivative of gap can be calculated from eq.(3.90) and (3.91). Fig.4.13 shows that there are three possible specific heat jump; c_{coex} to c_{CDW} and c_{coex} to c_n at T_s and c_{CDW} to c_n at T_c. As shown in chapter 3 the specific heat jump at T_c is exactly 1.43 as universal value of BCS theory. The first specific heat jump at T_s is defined by

$$\frac{\Delta c_1}{c_{CDW}} = \frac{c_{coex} - c_{CDW}}{c_{CDW}} \tag{4.33}$$

Figure 32 demonstrates the specific heat jump $\Delta c_1/c_{CDW}$ of the coexistence state as a function of T_{so}/T_c and T_s/T_{so}.

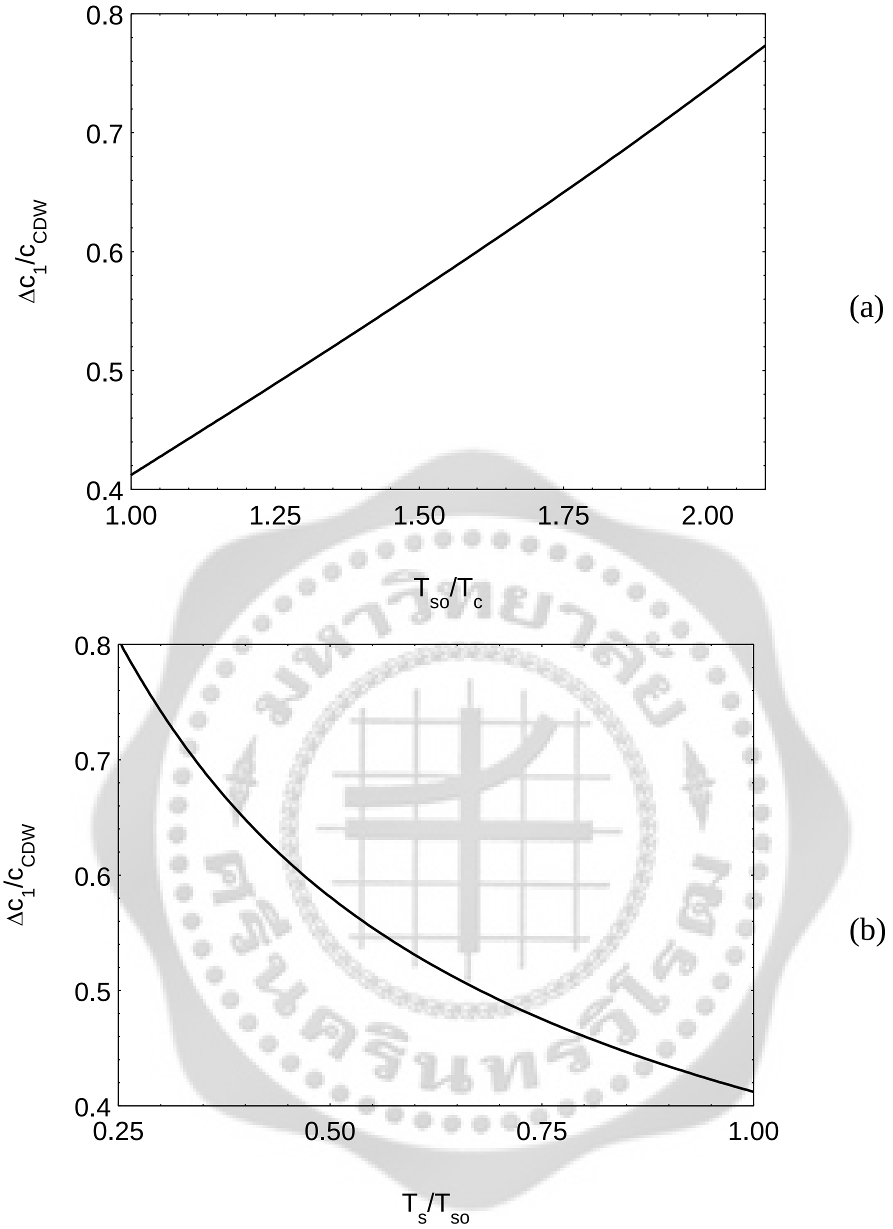


Figure 32 $\Delta c_1/c_{CDW}$ as a function of T_{so}/T_c (a) and T_s/T_{so} (b).

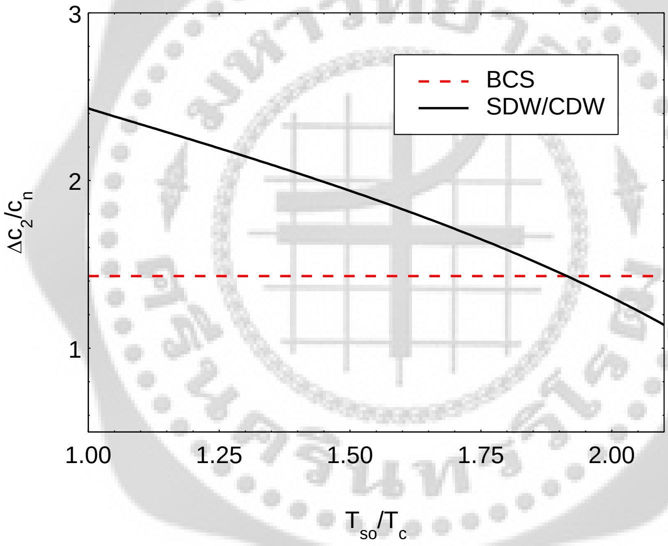
The specific heat jump is minimum with $\Delta c_1/c_{CDW}$ = 0.42 at T_{so}/T_c = 1= T_s/T_{so} which is rather smaller than 1.43. It increases with the increase in T_{so}/T_c or the decrease in T_s/T_{so}. If we calculate the specific heat jump compared to normal state at T_s

$$\frac{\Delta c_2}{c_n} = \frac{c_{coex} - c_n}{c_n}. \qquad (4.34)$$

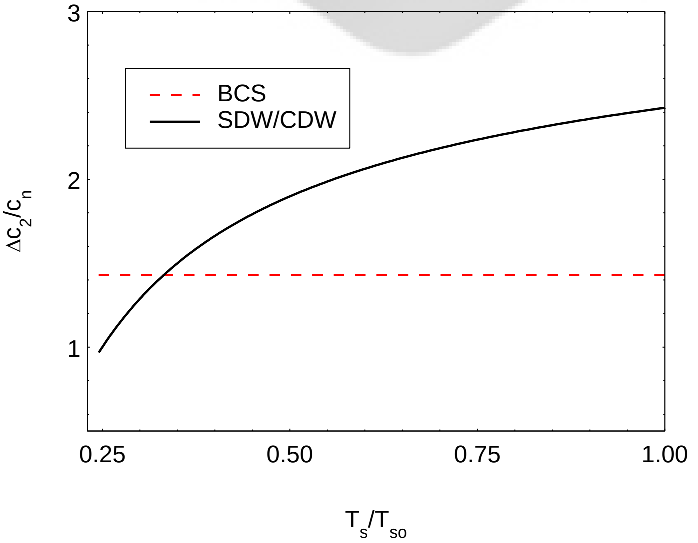
Its dependence on T_{so}/T_c and in T_s/T_{so} is shown in figure 33. In contrast to $\Delta c_1/c_{CDW}$ the specific heat jump $\Delta c_2/c_n$ decreases with the increase in T_{so}/T_c or the decrease in T_s/T_{so}. This specific heat jump can either greater than or less than the BCS value of 1.43. The observed specific heat jump for some of cuprate show that it deviates from the BCS value as shown in table 2. Some of them can be fitted with our calculation if we use T_s/T_{so} as an adjust parameter. For example, for specific heat jump 2.5 of YBCO7 match with our calculation at T_s/T_{so}~1.

Table 1 Specific Heat Jump $(\Delta c)/c_n$ at T_c (Plakida. 2010: 127)

Material	$(c-c_n)/c_n$
$YBCO_7$	2.5
$YBCO_{6.92}$	2.6
$(Y_{0.8}Ca_{0.2})BCO$	1.5
Bi-2212	1.3
Tl-2201	1.47
$(La_{1.86}Sr_{0.14})CO$	1.4
$(La_{1.78}Sr_{0.22})CO$	0.9



(a)



(b)

Figure 33 $\Delta c_2/c_n$ as a function of T_{so}/T_c (a) and T_s/T_{so} (b).

In order to compare the calculation to the experimental data, we consider the CDW state as a generalized case of SCstate. Figure 34 show the comparison between the calculation from eq.(4.6.4) and the experimental data of $Ba(Fe_{0.925}Co_{0.075})_2As_2$ (Vavilov; et al. 2011: 140502).

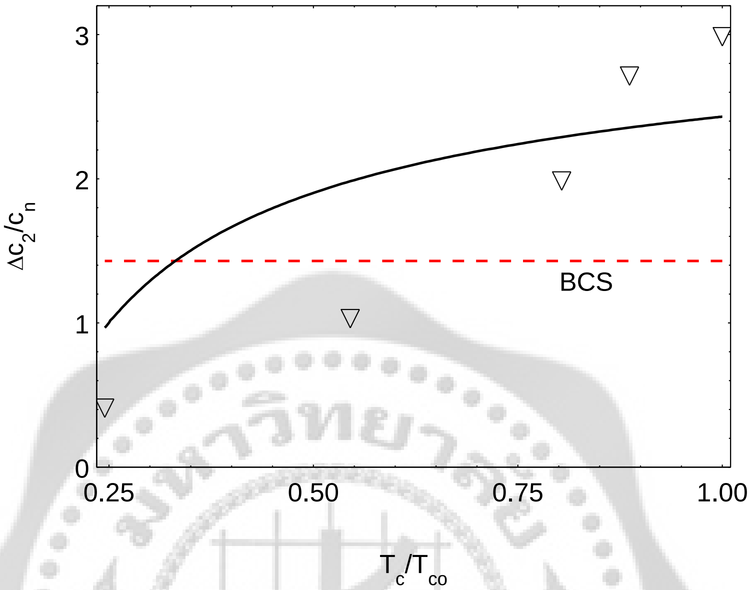


Figure 34 $\Delta c_2/c_n$as a function of T_c/T_{co} and experimental data of $Ba(Fe_{0.925}Co_{0.075})_2As_2$ (triangle).

It seems that our calculation shows the same tendency as experimental data. But it does not exactly fit with the data points.This would be due to our approximation assumption that W>>T in section 3.7. Many experiments performed on the HTS superconductor show that W/T is finite and might less than ten.

CHAPTER 5
CONCLUSIONS

In this research we study the effects of the interplay between SDW and CDW on the thermodynamic properties such as the energy gap, critical temperature and specific heat. We analyze the mean field Hamiltonian of the coexistence of SDW and CDW using Green's function method. The energy of the conduction electron or the energy dispersion is assumed be given by the tight binding model for two dimensional square lattice. To simplify the problem we consider only the hopping integral for the nearest neighborhood t_o and assumed that the chemical potential is zero. The self consistent gap equations of the coexistence state are derived from Green's function. From gap equations the thermodynamic properties of the coexistence state are calculated with the assumption that the band width is very large compared to gaps and density of state is constant near Fermi surface.

At zero temperature, the SDW and CDW gaps are calculated by introducing the gap ratio "a", which is depend on the coupling constants. The results show that both zero temperature gaps are suppressed by the interplay. The magnitude of the suppression is directly depends on the magnitude of the coupling constants. The suppression is so large for the state with the larger coupling constant. The coupling constant phase diagram shows that there are three regions; two regions for the pure SDW and CDW states and a region of the coexistence along a right diagonal line. The width of the coexistence region increases with increase in the magnitude of the coupling constant. At near zero temperature, the gap of the state with a larger coupling constant approach to its zero temperature increasingly. While the gap of the other state approach to its zero temperature gap decreasingly due to the interplay.

To obtain the expression of the critical temperature at the onset of the coexistence state, we assumed that the ratio of gap and critical temperature is less than a π and the band width is so large compared to that temperature. We obtain the expression of the critical temperature in term of the series of the of the gap and critical temperature times π. The results show the competition between SDW and CDW states, which depend on the magnitude of the coupling constants. The interplay suppresses the critical temperature of a state with a larger coupling constant. The critical temperature of a state with a smaller coupling constant does not effect by the interplay. It is same as that of the pure state. The temperature phase diagram shows two regions of the coexistence state and pure state separated by a phase boundary line. The transition to the coexistence state takes place when the system crosses this line. It also demonstrates that the critical temperature or the transition temperature of the onset of the coexistence state decreases with the increase in the different of the coupling constants. These explanations for the zero temperature gaps, the critical temperature and the phase diagram are well supported by our results of numerical solving of self consistent gap equation. However, our results about the critical temperature are rather in contrast with the previous work by Pradhan et at(Pradhan; et al. 2008:2332-2335). They show that the interplay between SDW and CDW can enhance the critical temperature of the state with a smaller coupling constant.The density of state and the band structure of the coexistence states show that there should be two effective gaps around the Fermi surface, which correspond to the sum and different of the SDW and CDW gaps. Our results show that the ratio of the zero temperature gap and the critical temperature at the onset of the coexistence state can be larger than that of the BCS universal value. These agree with some of the experimental data of cuprate and iron based superconductor. The gap-to-T_c ratio at the transition temperature from normal state to pure SDW or CDW state is exactly same as the BCS value.

At the onset of the coexistence state there are two possible specific heat jumps; jump from the coexistence state to pure state and to normal state. Our results show that only a specific heat jump for the coexistence state to normal state agree with the experimental data. It deviates from the typical value of the BCS jump. However, to compare with the experimental data of iron based superconductor $Ba(Fe_{0.925}Co_{0.075})_2As_2$, our calculations do not agree well with the experimental data. It only shows the same tendency. This might be due to the use of many approximations; especially the effect of the band width is not included in our calculation.

To improve or extend our study, it might be done as follow;

1. To consider the effect of the band width on the calculation because in the research we have usually assumed that the band width is very large compared to gap or temperature which we consider.

2. To account the effect from the next nearest neighbor in the energy of the conduction electrons the higher order of the hopping integral must be considered.

3. To make the calculation be more realistic, we might consider the momentum dependent interaction or the energy dependent density of states such as the van Hove DOS.

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