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Condensed Matter Core

# Homework 4

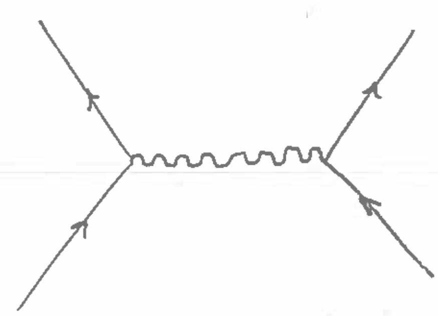
## 1. Summary of BCS Theory

A BCS superconductor is a condensate of Cooper pairs. These Cooper pairs consist of pairs of electrons. In particular, due to the addition of angular momentum $1/2 \otimes 1/2 = 0 \oplus 1$, they are bosonic and can form a condensate. In fact, in most cases, they belong to the spin singlet, so that the constituting electrons have opposite spin. In their ground state they have zero momentum. Thus, their constituting electrons have opposite momenta as well.

These pairs form due to attractive interactions between electrons whose energy is close to the Fermi level. In particular, these may very well be conducting electrons. The pairs then, even in their ground state may conduct. These conductance is protected by a pairing gap. This is an energy gap required to excite Bogoliubov fermions, i.e. to break Cooper pairs. This mechanism is responsible for the persistent currents found in these materials. At high enough temperatures however, thermal excitations are enough to overcome the pairing gap. Then the superconducting state is lost.

Other than the persistent current, an even more defining feature of superconductors is the Meissner effect. This consist of the ejection of a magnetic field from superconductors. This can be seen as a consequence of the Ginzburg-Landau description of BCS theory. In it, as a consequence of Spontaneous Symmetry Breaking, the vector potential becomes a massive field. Thus, it describes a short-ranged interaction. Therefore, magnetic fields vanish in the bulk.

Finally, a mechanism through which the attractive interaction appears is the electron-phonon interactions. Indeed, when an electron moves it creates a movement of the crystal. This in turn creates a movement of electrons, accounting for the effective electron-electron interaction



The help of Bruno, Gloria and Tales was very important.

2. d-wave superconductivity in high-$T_c$ cuprates

a) Under a ninety-degree passive rotation we have the new CAR generators

$$\tilde{c}_{i,\sigma} := c_{Ri,\sigma} ,$$

where $R$ is the $90°$ clockwise rotation matrix. We begin by noticing that

$$\Delta_{R^{-1}i, R^{-1}j} = - \Delta_{ij} .$$

Moreover, since $R$ is a bijection, for every function $f$ of two sites

$$\sum_{\langle i,j \rangle} f_{i,j} = \sum_{\langle i,j \rangle} f_{Ri, Rj} .$$

Thus, the pairing term is transformed to

$$\frac{1}{2}\sum_{\langle i,j\rangle}\left(\Delta_{i,j}\left(\tilde{c}_{i,\downarrow}\tilde{c}_{j,\uparrow}-\tilde{c}_{i,\uparrow}\tilde{c}_{j,\downarrow}\right)+h.c.\right)$$

$$=\frac{1}{2}\sum_{\langle i,j\rangle}\left(\Delta_{i,j}\left(c_{Ri,\downarrow}c_{Rj,\uparrow}-c_{Ri,\uparrow}c_{Rj,\downarrow}\right)+h.c.\right)$$

$$=\frac{1}{2}\sum_{\langle i,j\rangle}\left(\Delta_{R^{-1}Ri,R^{-1}Rj}\left(c_{Ri,\downarrow}c_{Rj,\uparrow}-c_{Ri,\uparrow}c_{Rj,\downarrow}\right)+h.c.\right)$$

$$=\frac{1}{2}\sum_{\langle i,j\rangle}\left(\Delta_{R^{-1}i,R^{-1}j}\left(c_{i,\downarrow}c_{j,\uparrow}-c_{i,\uparrow}c_{j,\downarrow}\right)+h.c.\right)$$

$$=\frac{1}{2}\sum_{\langle i,j\rangle}\left(-\Delta_{i,j}\left(c_{i,\downarrow}c_{j,\uparrow}-c_{i,\uparrow}c_{j,\downarrow}\right)+h.c.\right)$$

$$=-\frac{1}{2}\sum_{\langle i,j\rangle}\left(\Delta_{ij}\left(c_{i,\downarrow}c_{j,\uparrow}-c_{i,\uparrow}c_{j,\downarrow}\right)+h.c.\right),$$

i.e., the negative of itself.

b) Let us assume we have periodic boundary conditions, so that the lattice has $L_x \times L_y$ sites. Then, for every function $f$ on the lattice we have that for $k \in \underbrace{\left( \frac{2\pi}{L_x} \mathbb{Z}/_{L_x \mathbb{Z}} \right) \times \left( \frac{2\pi}{L_y} \mathbb{Z}/_{L_y \mathbb{Z}} \right)}_{}$ $\overset{\tilde{\Lambda}}{\underset{!!}{}}$

$$\tilde{f}_k := \frac{1}{\sqrt{N}} \sum_{i \in \Lambda} e^{-ik\cdot i} f_i$$

$$\Lambda = \mathbb{Z}/_{L_x \mathbb{Z}} \times \mathbb{Z}/_{L_y \mathbb{Z}}$$

contains all information on $f$. Indeed

$$\frac{1}{\sqrt{N}} \sum_{k \in \tilde{\Lambda}} e^{ik\cdot i} \tilde{f}_k = \frac{1}{N} \sum_{k \in \tilde{\Lambda}, j \in \Lambda} e^{ik\cdot(i-j)} f_j$$

$$= \sum_{j \in \Lambda} \delta_{i,j} f_j = f_i .$$

Therefore,

$$\sum_{\langle ij \rangle} c^+_{i,\sigma} c_{j,\sigma} = \frac{1}{N} \sum_{\substack{\langle ij \rangle, \\ k,q \in \tilde{\Lambda}}} e^{i(-k\cdot i + q\cdot j)} c^+_{k,\sigma} c_{q,\sigma}$$

$$= \frac{1}{N} \sum_{i \in \Lambda,\, k,q \in \tilde{\Lambda},\, \mu \in \{1,2\}} e^{i(q-k)\cdot i} e^{iq\cdot e_\mu} c^+_{k,\sigma} c_{q,\sigma}$$

$$= \sum_{k,q\in\tilde{\Lambda}} \delta_{k,q} \sum_{\mu\in\{1,2\}} e^{iq\cdot e_\mu} c^+_{k,\sigma} c_{q,\sigma}$$

$$= \sum_{k\in\tilde{\Lambda}} \left( e^{ik_x} + e^{ik_y} \right) c^+_{k,\sigma} c_{k,\sigma}.$$

Thus, the hopping term is

$$-t \sum_{\langle ij\rangle} \sum_{\sigma} \left( c^+_{i,\sigma} c_{j,\sigma} + h.c. \right)$$

$$= -t \sum_{k} \sum_{\sigma} \left( e^{ik_x} + e^{ik_y} + e^{-ik_x} + e^{-ik_y} \right) c^+_{k,\sigma} c_{k,\sigma}$$

$$= -2t \sum_{k,\sigma} \left( \cos(k_x) + \cos(k_y) \right) c^+_{k,\sigma} c_{k,\sigma}.$$

The chemical potential term is

$$-\mu \sum_{i,\sigma} c^+_{i,\sigma} c_{i,\sigma} = -\frac{\mu}{N} \sum_{i,\sigma,k,q} e^{i(q-k)\cdot i} c^+_{k,\sigma} c_{q,\sigma}$$

$$= -\mu \sum_{\sigma,k,q} \delta_{q,k} c^+_{k,\sigma} c_{q,\sigma} = -\mu \sum_{k,\sigma} c^+_{k,\sigma} c_{k,\sigma}.$$

Finally, the pairing term is

$$\frac{1}{2N} \sum_{\langle ij \rangle, k, q} \left( \Delta_{ij}\, e^{i(k\cdot i + q\cdot j)} \left(c_{k,\downarrow} c_{q,\uparrow} - c_{k,\uparrow} c_{q,\downarrow}\right) + h.c. \right)$$

$$= \frac{1}{2N} \sum_{i,\sigma,k,q,\mu} \left( (-1)^{\mu+1} \Delta_0\, e^{i(k+q)\cdot i}\, e^{iq\cdot e_\mu} \left(c_{k,\downarrow} c_{q,\uparrow} - c_{k,\uparrow} c_{q,\downarrow}\right) + h.c. \right)$$

$$= \frac{\Delta_0}{2} \sum_{\sigma,k,q,\mu} \left( (-1)^{\mu+1}\, e^{iq\cdot e_\mu}\, \delta_{k,-q} \left(c_{k,\downarrow} c_{q,\uparrow} - c_{k,\uparrow} c_{q,\downarrow}\right) + h.c. \right)$$

$$= \frac{\Delta_0}{2} \sum_{k,\sigma} \left( \left(e^{-ik_x} - e^{-ik_y}\right)\left(c_{k,\downarrow} c_{-k,\uparrow} - c_{k,\uparrow} c_{-k,\downarrow}\right) + h.c. \right)$$

$$= \frac{\Delta_0}{2} \sum_{k,\sigma} \left( \left(e^{-ik_x} - e^{-ik_y}\right)\left(c_{k,\downarrow} c_{-k,\uparrow} + c_{-k,\downarrow} c_{k,\uparrow}\right) + h.c. \right)$$

$$= \frac{\Delta_0}{2} \sum_{k,\sigma} \left( \left(e^{-ik_x} - e^{-ik_y}\right) c_{k,\downarrow} c_{-k,\uparrow} + \left(e^{ik_x} - e^{ik_y}\right) c_{k,\downarrow} c_{-k,\uparrow} + h.c. \right)$$

$$= \Delta_0 \sum_{k,\sigma} \left( \left(\cos(k_x) - \cos(k_y)\right) c_{k,\downarrow} c_{-k,\uparrow} + h.c. \right).$$

(Dalila showed me the final result of this calculation).

We thus have

$$H = \sum_{k,\sigma} \Big( \big(-2t(\cos(k_x)+\cos(k_y)) - \mu\big) c^{+}_{k,\sigma} c_{k,\sigma}$$

$$+ \Delta_0(\cos(k_x)-\cos(k_y))\big(c_{k,\downarrow} c_{-k,\uparrow} + c^{+}_{-k,\uparrow} c^{+}_{k,\downarrow}\big)\Big)$$

$$= \sum_{k} \Big( \big(-2t(\cos(k_x)+\cos(k_y)) - \mu\big)\big(c^{+}_{k,\uparrow} c_{k,\uparrow} + c^{+}_{k,\downarrow} c_{k,\downarrow}\big)$$

$$+ \Delta_0(\cos(k_x)-\cos(k_y))\big(c^{+}_{k,\uparrow} c^{+}_{-k,\downarrow} + c_{k,\downarrow} c_{-k,\uparrow}\big).$$

The interaction term begs the spinor

$\Phi_k = \begin{pmatrix} c_{k,\uparrow} \\ c^{+}_{-k,\downarrow} \end{pmatrix}$. Setting $h_k = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$

we have

$$\sum_{k} \Phi^{+}_{k} h_k \Phi_k = \sum_{k}\big(a\, c^{+}_{k,\uparrow} c_{k,\uparrow} + b\, c^{+}_{k,\uparrow} c^{+}_{-k,\downarrow} + c\, c_{-k,\downarrow} c_{k,\uparrow}$$

$$+ d\, c_{-k,\downarrow} c^{+}_{-k,\downarrow}\big)$$

$$= \sum_{k}' \Big( a\, c_{k,\uparrow}^{+} c_{k,\uparrow} - d\, c_{k,\downarrow}^{+} c_{k,\downarrow}$$

$$+ b\, c_{k,\uparrow}^{+} c_{-k,\downarrow}^{+} + c\, c_{-k,\downarrow} c_{k,\uparrow} + d \Big).$$

We thus see

$$H = \sum_{k}' \Phi_k^{+} h_k \Phi_k \quad + \text{constant} \quad \text{with}$$

$$a = -d = -2t\,(\cos(k_x) + \cos(k_y)) - \mu$$

$$b = c = \Delta_0\,(\cos(k_x) - \cos(k_y)).$$

Dalila helped me a lot!

c) For such a matrix the characteristic polynomial is

$$p(\lambda) = (a - \lambda)(-a - \lambda) - b^2$$

$$= \lambda^2 - a^2 - b^2 = \left(\lambda - \sqrt{a^2 + b^2}\right)\left(\lambda + \sqrt{a^2 + b^2}\right).$$

We thus see that the dispersion relation is

$$\pm E_{\vec{k}} = \pm \sqrt{a^2 + b^2} .$$

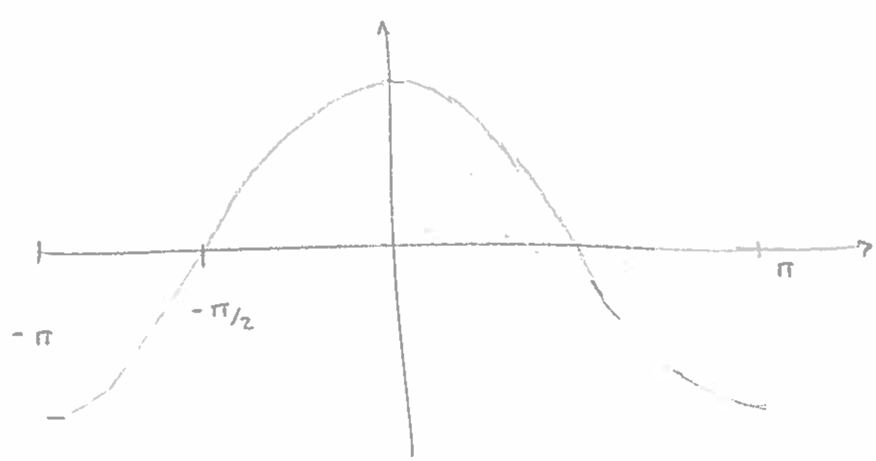
Since under a $90^\circ$ rotation

$$b \longmapsto \Delta_0 (\cos(k_y) - \cos(-k_x)) = -b,$$

we let $\Delta_{\vec{k}} = b$ and $\xi_{\vec{k}} = a$.

d) Clearly, the momenta at which the gap vanishes is given by

$$\cos(k_x) = \cos(k_y) .$$



By looking at this graph, we see that this only happens at

$$|k_x| = |k_y|.$$

The plot is found in the next page. The zeroes are plotted in blue.

c) We have

$$E_{\vec{k}} = \sqrt{4t^2 \left(\cos(k_x) + \cos(k_y)\right)^2 + \Delta_0^2 \left(\cos(k_x) - \cos(k_y)\right)^2}$$

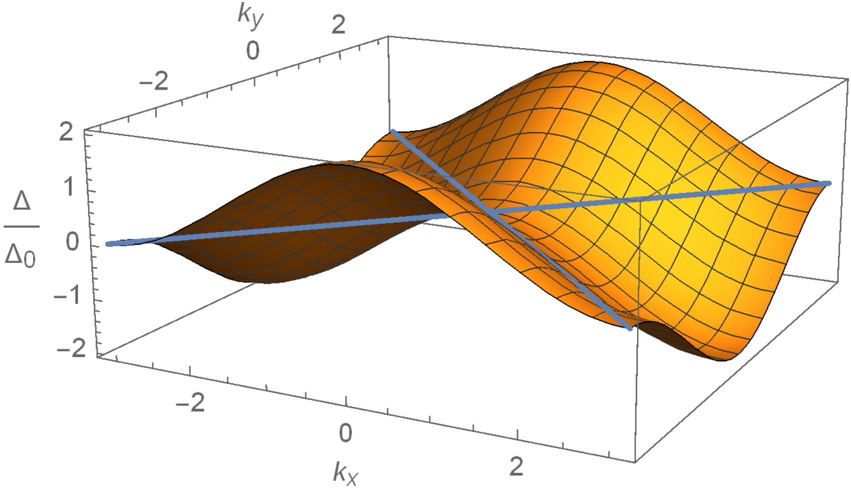
clearly vanishes only if

$$\cos(k_x) = -\cos(k_y) = -\cos(k_y).$$

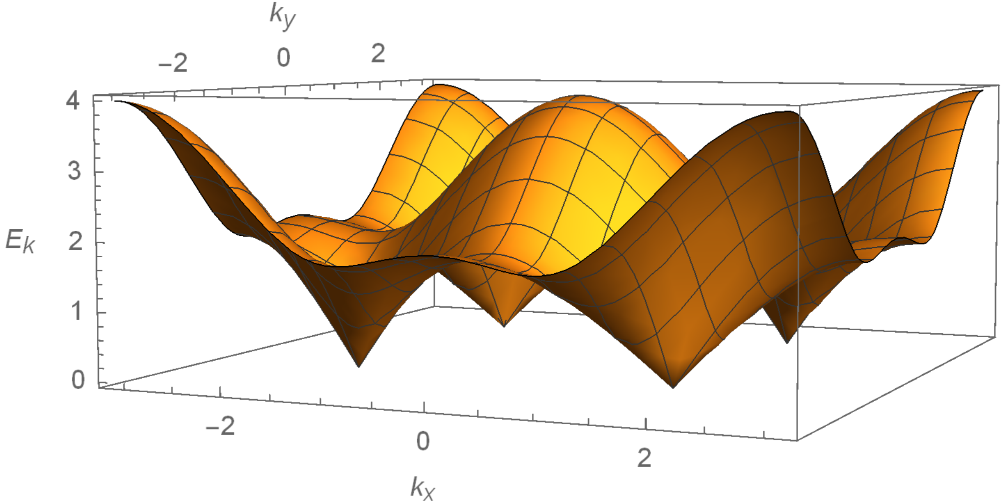
Thus $\cos(k_x) = 0$ and $|k_x| = |k_y|$, i.e.

$$k \in \{(-\pi/2, -\pi/2), (-\pi/2, \pi/2), (\pi/2, -\pi/2), (\pi/2, \pi/2)\}.$$

The graph is found in the next page.



$k_y$
2
0
−2
2
1
$\frac{\Delta}{\Delta_0}$
0
−1
−2
−2
0
2
$k_x$



$k_y$
−2
0
2
4
3
2
1
0
$E_k$
−2
0
2
$k_x$

f) Since we are at Half-filling, the Fermi surface corresponds to the momentas where the gap vanishes. As argued before, these are given by the cross

$$|k_x| = |k_y|.$$

Now, let us focus on the node $(\pi/2, \pi/2)$. The component parallel to the Fermi surface at this point is

$$k_1 = (\delta k_x, \delta k_y) \cdot \left(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right) = \frac{1}{\sqrt{2}}(\delta k_x + \delta k_y).$$

On the other hand, the perpendicular component is

$$k_2 = (\delta k_x, \delta k_y) \cdot \left(-\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right) = \frac{1}{\sqrt{2}}(-\delta k_x + \delta k_y).$$

In other words

$$\delta k_x = \frac{1}{\sqrt{2}} (k_1 - k_2)$$

$$\delta k_y = \frac{1}{\sqrt{2}} (k_1 + k_2).$$

Thanks to Janos and Gloria for intuition on Fermi surface

We then have that near the node

$$E_k = \pm \sqrt{4t^2 \left(\cos\left(\frac{\pi}{2} + \frac{1}{\sqrt{2}}(k_1 - k_2)\right) + \cos\left(\frac{\pi}{2} + \frac{1}{\sqrt{2}}(k_1 + k_2)\right)\right)^2}$$

$$\overline{+ \Delta_o^2 \left(\cos\left(\frac{\pi}{2} + \frac{1}{\sqrt{2}}(k_1 - k_2)\right) - \cos\left(\frac{\pi}{2} + \frac{1}{\sqrt{2}}(k_1 + k_2)\right)\right)^2}$$

$$= \pm \sqrt{4t^2 \left(\sin\left(\frac{1}{\sqrt{2}}(k_1 - k_2)\right) + \sin\left(\frac{1}{\sqrt{2}}(k_1 + k_2)\right)\right)^2}$$

$$\overline{+ \Delta_o^2 \left(\sin\left(\frac{1}{\sqrt{2}}(k_1 - k_2)\right) - \sin\left(\frac{1}{\sqrt{2}}(k_1 + k_2)\right)\right)^2}$$

$$= \pm \sqrt{4t^2 \left(\frac{1}{\sqrt{2}}(k_1 - k_2) + \frac{1}{\sqrt{2}}(k_1 + k_2) + \mathcal{O}\left((k_1, k_2)^2\right)\right)^2}$$

$$\overline{+ \Delta_o^2 \left(\frac{1}{\sqrt{2}}(k_1 - k_2) - \frac{1}{\sqrt{2}}(k_1 + k_2) + \mathcal{O}\left((k_1, k_2)^2\right)\right)^2}$$

$$= \pm \sqrt{8t^2 k_1^2 + 2\Delta_o^2 k_2^2}\,.$$

Thus $v_F = 2\sqrt{2}\, t$ and $v_\Delta = \sqrt{2}\, \Delta_o$.

3. Landau mean-field theory

a) For the BCS superconductor $\Delta$ corresponds to the pairing gap, as explained in 1. During the lectures we saw that $\Delta$ could always be taken as real by redefining the CAR generators. This reflects a $U(1)$ symmetry. Thus $f$ can only be a function of $|\Delta|$. However, in light of (6), it has to be analytic in $\Delta$. Since $|\Delta|$ is not, $f$ must be a function of $|\Delta|^2$. Thus

$$f = a|\Delta|^2 + b|\Delta|^4 + \cdots .$$

b) Another system with the same Landau free energy would be the $O(2)$ model. In it the order parameter is the magnetization $\vec{M} \in \mathbb{R}^2$. This is invariant under rotations. The discussion between both models becomes identical under the identification

$$\mathbb{R}^2 \longmapsto \mathbb{C}.$$

In particular, under this $O(2) \longmapsto U(1)$.

Although these two theories have a very different, and seemingly unrelated, microscopic behaviour, they posses the same symmetries.

Therefore, they have the same Landau theoretic description. The success of Landau theory exemplifies then the concept universality. Models with different microscopic origins may develop the same critical behaviour.

c) We have

$$\frac{df}{d|\Delta|} = 2a|\Delta| + 4b|\Delta|^3 = 2|\Delta|\left(a + 2b|\Delta|^2\right).$$

Thus, the critical locus of $f$ is the set of $\Delta$ s.t. $|\Delta| \in \{0\} \cup \{\Delta_0 \mid a + 2b|\Delta|^2 = 0\}$.

If $a > 0$, i.e. if $T > T_c$, the latter is clearly empty. Then $\Delta_0 = 0$. If $a < 0$, i.e. if $T < T_c$, we have that the critical locus are the $\pm |\Delta|$ s.t.

$$|\Delta| \in \{0, \pm\sqrt{-a/2b}\}.$$

For $|\Delta| = 0$, $f = 0$. However, if

$$|\Delta| = \pm\sqrt{-a/2b},$$

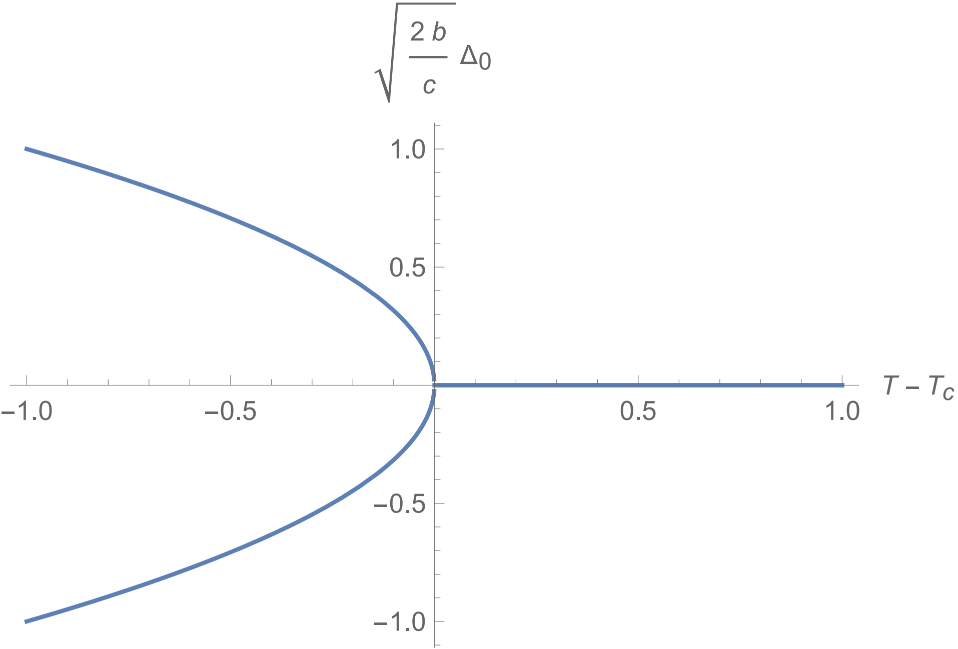
$$f = a\left(-\frac{a}{2b}\right) + b\left(-\frac{a}{2b}\right)^2$$

$$= -\frac{a^2}{2b} + \frac{a^2}{4b} = -\frac{a^2}{4b} < 0.$$

Thus, $\Delta_0 = \pm\sqrt{-a/2b}$. The plot is found on the next page. In particular

$$\Delta_0 \propto \sqrt{-a} \propto \sqrt{T_c - T},$$

s.t. $\beta = 1/2$.



$\sqrt{\frac{2b}{c}}\Delta_0$
1.0
0.5
−0.5
−1.0
$T - T_c$
−1.0
−0.5
0.5
1.0

d) For $T > T_c$, $F = 0$ so $C = 0$. On the other hand, for $T < T_c$

$$F = -\frac{a^2}{4b} = -\frac{c^2}{4b}(T - T_c)^2 .$$

Thus

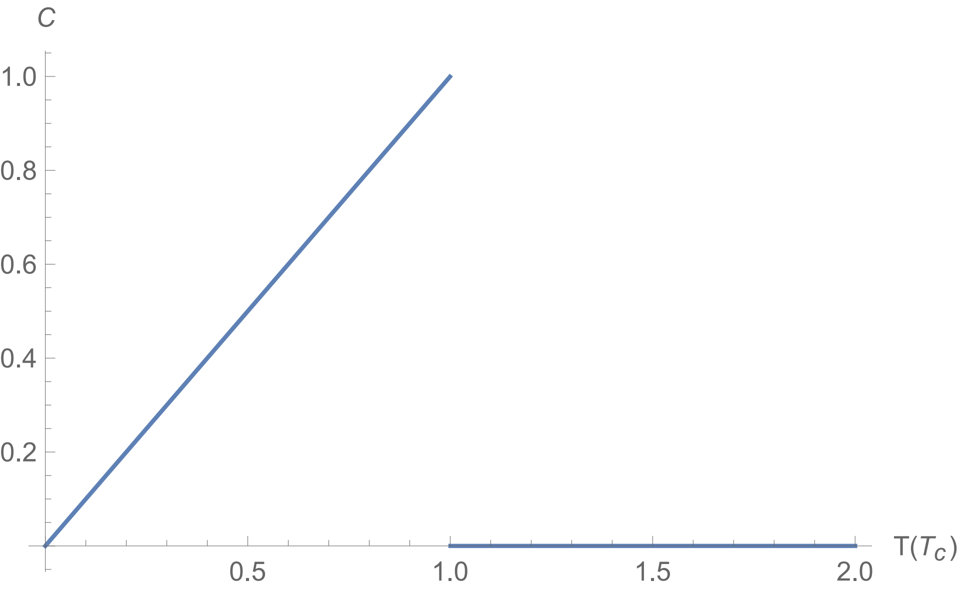
$$C = -T\frac{\partial^2 f}{\partial T^2} = \frac{c^2}{4b} 2T = \frac{c^2}{2b}\left[(T - T_c) + T_c\right] \approx \frac{c^2}{2b} T_c$$

We conclude $\alpha = 0$.

We have

$$C((T - T_c) \to 0^+) - C((T - T_c) \to 0^-)$$

$$= 0 - \lim_{T \to T_c^-} \frac{c^2}{2b} T = -\frac{c^2}{2b} T_c .$$


C
1.0
0.8
0.6
0.4
0.2
0.5
1.0
1.5
2.0
T(T_c)

e) The plot is shown in the next page.

It was obtained from

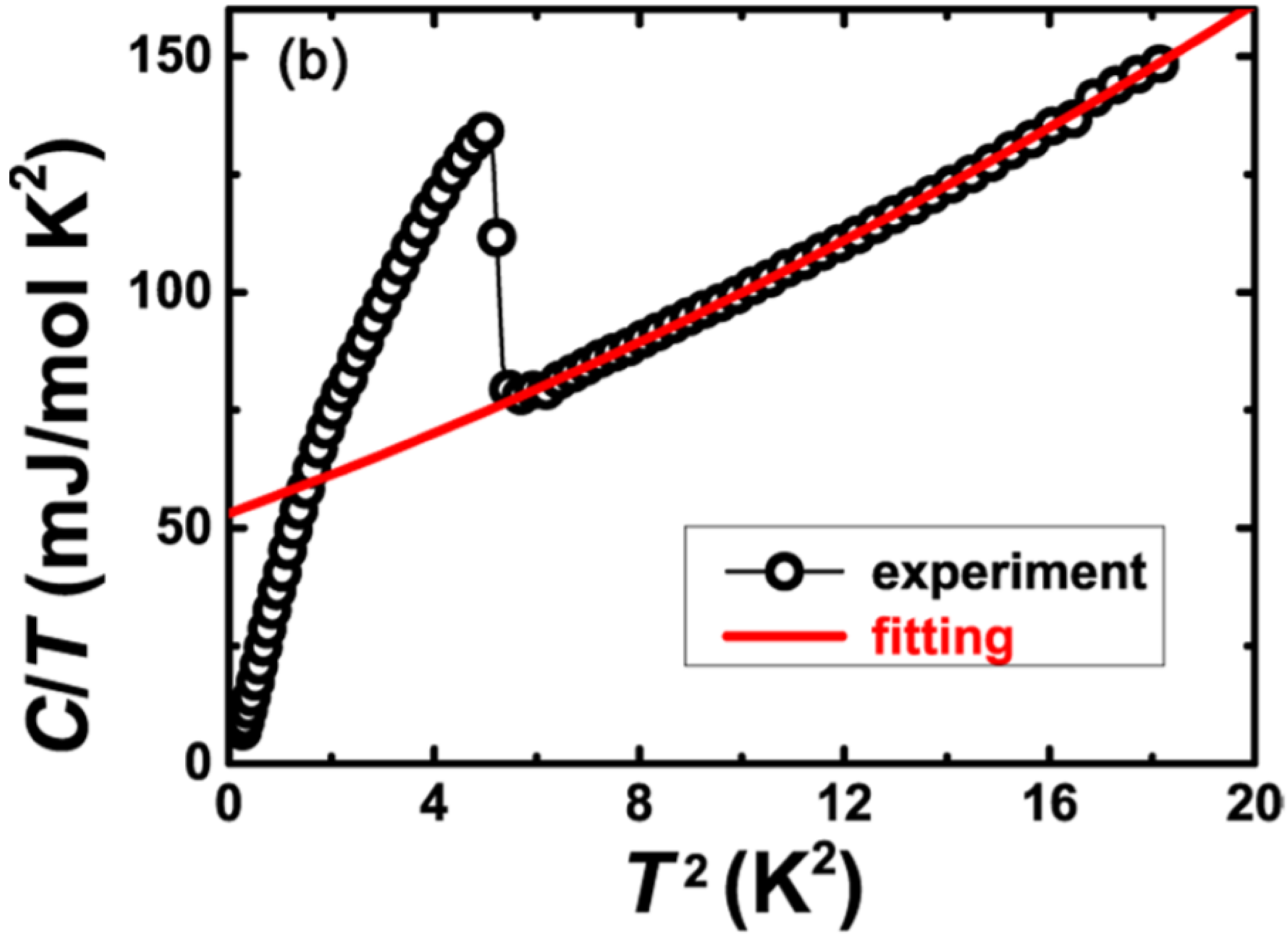
Li, B., Xu, C.Q., Zhou, W. et al. Evidence of s-wave superconductivity in the noncentrosymmetric $La_7Ir_3$. Sci Rep 8, 651 (2018) doi: 10.1038/s41598-017-19042-x

Much like in our predictions, there is a discontinuity at a critical temperature. However, our result is

$$\frac{C}{T} = \begin{cases} \frac{c^2}{2b} > 0 & T < T_c \\ 0 & T > T_c, \end{cases}$$

which is very different from the curve observed.

T (K)



In particular, this curve has no obvious constant regions.

f) Allowing for fluctuations we can draw inspiration from a complex scalar field theory

$$f = C\|\nabla\Delta\|^2 + a|\Delta|^2 + b|\Delta|^4 + \cdots,$$