Weak coupling theories of unconventional superconductivity (I)

(Superconductivity from repulsion)

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Superconductivity:

Zero-resistance state of interacting electrons



Let's start with some basics:

Consider a system of fermions with k²/2m dispersion and (screened) Coulomb interaction U(r).

Single-particle (fermionic) excitations are described by the poles of the fermionic Green's function $G(k, \omega)$

For free fermions, $G(k, \omega) = 1/(\omega - v_F (k-k_F))$

In a Fermi liquid, $G(k, \omega) = Z/(\omega - v_F^*(k-k_F))$

Superconductivity is a two-particle instability of a system of interacting fermions

Collective two-particle (bosonic) excitations are described by the poles of the vertex function $\Gamma(q,\Omega)$ =fully renormalized interaction

Examples: sound (or zero sound) waves in a Fermi liquid

If Γ (q, Ω) had a pole in the upper half-plane, perturbations would increase with time and eventually destroy a Fermi liquid

Superconducting instability is of this kind

To first order in the interaction, Γ (q, Ω) is just an antisymmetrized interaction – no poles!



Roughly, $\Gamma = -\mathbf{U}$

$$\Gamma = U(k_1 - k_4) \delta_{dS} \delta_{\beta} - U(k_1 - k_3) \delta_{dJ} \delta_{\beta} S$$

$$= \frac{1}{2} \left[U(k_1 - k_4) + U(k_1 - k_3) \right] \left(\delta_{ab} \delta_{b} - \delta_{ab} \delta_{b} \right) \quad \text{singlet}$$

+
$$\frac{1}{2} \left[U(k_1 - k_2) - U(k_1 - k_3) \right] \left(\delta_{\alpha \delta} \delta_{\beta j} + \delta_{\alpha j} \delta_{\beta \delta} \right)$$
 triplet

Let's now include higher-order terms:



For generic momenta, a boring perturbation theory, but if total incoming momenta and frequency are zero, there is a singularity





And keep adding singular particle-particle renormalizations



Integral equation on the full vertex

Take $\Gamma_0 = \text{const} \ (\Gamma_0 = - \text{ U in the Hubbard model})$

$$\Gamma = \frac{\Gamma_{o}}{1 - \Gamma_{o} N_{F} \left[\log \frac{\Lambda}{|\mathcal{P}|} + \frac{i N_{F}}{2} \right]}$$
For repulsive
interaction, Γ_{0}
is negative, and
But if $\Gamma_{0} > 0$
(attraction)
 $\Gamma \simeq \frac{1}{\mathcal{R} - i \mathcal{R}_{o}} \qquad \mathcal{R}_{o} = \Lambda \stackrel{-}{\in} \frac{1}{\Gamma_{o} N_{F}}$

Pole in the upper frequency half-plane, i.e., perturbations grow with time and destroy the normal state

[s

This is true only at small total momentum

$$\frac{1}{\mathcal{R} - i \mathcal{R}_0 \left(1 - \frac{V_F^2 q^2}{6 \mathcal{R}_0^2}\right)}$$

Superconductivity from repulsive interaction

How one possibly get $\Gamma_0 > 0$ out of repulsion?





Lev Landau

What if Γ_0 is a function of momentum?

 $[c_{i}(\vec{k},\vec{p})) = |\vec{k}| = PF$ $|\vec{p}| = PF$



Lev Pitaevskii

$$\Gamma_{0}(\Theta) = \sum_{\ell=0}^{\infty} (2\ell+1) \Gamma_{\ell,0} P_{\ell}(\cos\Theta)$$
$$\Gamma'(\Theta) = \sum_{\ell=0}^{\infty} (2\ell+1) \Gamma_{\ell} P_{\ell}(\cos\Theta)$$

 \cap

Different angular harmonics decouple

$$= \frac{\Gamma_{e,0}}{1 - \Gamma_{e,0} N_F \left[\log \frac{\Lambda}{|J^2|} + \frac{i N_Z}{2} \right]}$$

It is sufficient to have $\Gamma_{1,0} > 0$ for just one value of l

ſ,



Walter Kohn

Kohn-Luttinger mechanism 1965

Components of the interaction with large lcome from large distances. At such distances, bare repulsive interaction occasionally gets over- screened and acquires oscillations $[U(r) = \cos (2k_F r)/r^3],$ often called Friedel oscillations



Joaquin Luttinger



How this actually works?



Particle-hole polarization bubble has a non-analyticity at $2p_F$ (i.e., at $\theta=0$)

$$\Pi \left(2p_F + x \right) - \Pi \left(2p_F \right) \sim x \log x$$

Because of non-analyticity, components $\Gamma_{l>>1}$ decay by a power-law, as $1/l^4$

$$\Gamma_{l>>1} = U^2 N_F / (2l^4) > 0$$

Components of the screened Coulomb interaction with large l are attractive, independent on the parity of l



Later developments:

Fay&Layzer, Kagan&A.C...

The attraction extends down to l=1, and Γ_1 is the largest:

 $\Gamma_1 = U^2 (2 \log 2 - 1) > 0$ p-wave instability

There is no interference with the bare U because bare U only contributes to s-wave channel

If U=U(q), situation is different, one needs to overcome bare $U_{l=1}$

However, $U_{l=1} \sim p_{F,}^2$ while the second order term $\sim p_{F,}$ and it definitely wins at low density

Kohn and Luttinger applied their result to 3He

At that time (1965) the general belief was that the pairing in 3He must be d-wave (l=2)

KL obtained Tc ~ $E_F \exp [-2.5 l^4]$, substituted l=2, and found Tc~ 10⁻¹⁷ K

A few years later it was found that l=1 for ³He.

Tc (l=1) ~ 10^{-3} E_F ~ 10^{-3} K (Tc ~ 3 mK in ³He)

I will focus on 2D systems for the rest of the lectures

Kohn-Luttinger effect in 2D

 $\Gamma_0(\theta) = -U^2 \Pi (2p_F \cos \theta/2)$

 $\Pi (q < 2p_F) = m/(2\pi) = const$



No superconductivity at this stage

Two ways to extend the analysis:

I. Go to higher order in U (U³)



Two ways to extend the analysis:

To order U³



Attraction again persists down to l=1, and $\Gamma_{l=1}$ is the largest

p-wave instability in a 2D isotropic Fermi liquid

Two ways to extend the analysis:

II. Do calculations on a lattice, with full E(k)





Details matter, but most likely outcome is d-wave

(Raghu's lectures)



For the rest of the lectures I will explore KL idea that the effective pairing interaction is different from a bare repulsive U due to screening by other fermions, and it may have attractive components in some channels

•cuprates

- doped graphene
- Fe-pnictides

Each case will represent different lattice version of KL physics

Cuprates (1986...)



Fig. 1. Evolution of the superconductive transition temperature subsequent to the discovery of the phenomenon.



 $YBa_2Cu_3O_{6+x}$



Phase diagram



Parent compounds are antiferromagnetic insulators

Superconductivity emerges upon either hole or electron doping

Overdoped compounds are metals and Fermi liquids

 $TI_2Ba_2CuO_{6+\delta}$ Nd_{2-x}Ce_xCuO₄ La_{2-x}Sr_xCuO₄ 300 Temperature (K) "Normal" 200 Metal Pseudogap 100 AF AF SC 0.3 0.2 0.1 0.00.2 0.3 0.1Dopant Concentration x

Overdoped compounds are metals and Fermi liquids

 $TI_2Ba_2CuO_{6+\delta}$

Photoemission





Areas are consistent with Luttinger count for electrons in a Fermi liquid

Overdoped compounds are metals and Fermi liquids

 $TI_2Ba_2CuO_{6+\delta}$



Oscillations in magnetoresistance

Vignolle et al

Areas are consistent with Luttinger count for electrons in a Fermi liquid

Fermi surface



Hole-dopedElectron-doped $E(k) = -2t (\cos kx + \cos ky) + 4t' \cos kx \cos ky - \mu$

For a square lattice, the symmetry group is D_{4h}

$$X \leftrightarrow Y \text{ and } X, Y \leftrightarrow -X, -Y$$



Kohn-Luttinger-type consideration



We have repulsive interactions within a patch and between patches

Consider Hubbard U

To first order, we only have a repulsive s-wave component.

To order U²





Let's momentarly consider only a larger $\Gamma_0(1,2)$



Let's momentarly consider only a larger $\Gamma_0(1,2)$



Let's momentarly consider only a larger $\Gamma_0(1,2)$



Doped graphene

Graphene -- an atomic-scale honeycomb lattice made of carbon atoms.









$$\varepsilon(k) = t_1 \sqrt{1 + 4\cos\frac{k_y \sqrt{3}}{2}\cos\frac{3k_x}{2} + 4\cos^2\frac{k_y \sqrt{3}}{2}} - \mu$$

$$\mu = 0$$
, Dirac points

$$\mu = t_1$$
, van Hove points





E. Rotenberg et al PRL 104, 136803 (2010)





$$\Gamma_0(1,1) = \Gamma_0(2,2) = \Gamma_0(3,3) = g_4$$

$$\Gamma_0(1,2) = \Gamma_0(2,3) = \Gamma_0(1,3) = g_3$$






$$\Gamma_0(1,1) = \Gamma_0(2,2) = \Gamma_0(3,3) = g_4$$

$$\Gamma_0(1,2) = \Gamma_0(2,3) = \Gamma_0(1,3) = g_3$$

$$\Gamma_{c;0} = -g_4 - 2g_3, \quad \Gamma_{a,b;0} = -g_4 + g_3,$$

need $\Gamma > 0$ for pairing

Do Kohn-Luttinger analysis:

Consider Hubbard U

To first order in U, $g_4=g_3=U$, and we only have a repulsive s-wave component $\Gamma_{c,0} < 0$, $\Gamma_{a,b,0} = 0$



 $\Gamma_0(1,2) > \Gamma_0(1,1)$, i.e., g3 > g4 and $\Gamma_{a,b;0} > 0$





The two d-wave solutions are degenerate by symmetry

Gonzales

Landau-Ginzburg expansion

 $F = \alpha (T - T_c) (|\Delta_a|^2 + |\Delta_b|^2) + K_1 (|\Delta_a|^2 + |\Delta_b|^2)^2 + K_2 |\Delta_a^2 + \Delta_b^2|^2 + O(\Delta^6)$

d+id state wins

chiral superconductivity (phase winds up by 4π)



chiral superconductivity (phase winds up by 4π)

Weakly/moderately doped systems:



New breakthrough in 2008: Fe-pnictides

LaFeAsO_{1-x}
$$F_x$$
, Tc = 26K
SmFeAsO_{1-x} F_x , Tc = 43K



Hideo Hosono

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X. H. Chen <u>ı (#ai)</u> , T. Wu <u>ı (#ai)</u>	
1. Hefei National Laboratory for Phys Letter	of science
Correspondence to: X. H. Chen1(#1). Nature 459, 64-67 (7 May 2009) doi:10.1038/nature07981; Received 4 November 2008; Accepted 13 March 2009	Search This journalgo_Advanced search
Since the discovery of hig been devoted to exploring A large iron isotope effect in SmFeAsO _{1 - X} F _X and Ba _{1 - X} K _X Fe ₂ As ₂ from Bardeen-Cooper-St copper oxide supercondut (ref. <u>2(/nature/journal/v455</u>) R. H. Liu ⁴ , T. Wu ⁴ , G. Wu ⁴ , H. Chen ⁴ , X. F. Wang ⁴ , Y. L. Xie ⁴ , J. J. Ying ⁴ , Y. J. Yan ⁴ , Q. J. Li ⁴ , B. C. Shi ⁴ , W. S. Chu ²⁺² , Z. Y. Wu ²⁺² & X. H. La-Nd, Sm and Gd) are no Chen ⁴	Accepted 5 May 2008; Published online 4 June 2008 ;F0.15
LaO _{1-x} F _x FeAs (ref. <u>2 (/nat</u> superconductivity in the r measurements reveal atr 3. National Synchrotron Radiation Facility, Institute of High Energy Physics, Chinese Academy of Sciences, Beijing 100049, China 3. National Synchrotron Radiation Laboratory, University of Science and Technology of China, Hefei 200049, China	& C. L. Chien <u>1 (#a1)</u> 1218, USA xc3, University of Science and Technology of China, Hefei, Anhui 230026, China

Band theory calculations for Fe-pnictides agree with experiments

Lebegue, Mazin et al, Singh & Du, Cvetkovic & Tesanovic...



2-3 circular hole pockets around (0,0)

2 elliptical electron pockets around (π,π) (folded BZ), or $(0,\pi)$ and $(\pi,0)$ (unfolded BZ)

A toy model: one hole and one electron pocket



$$\Gamma_{a,0} = -g_3 - g_4,$$

$$\Gamma_{b,0} = g_3 - g_4,$$

$$\Gamma > 0 \text{ is needed for SC}$$

Do Kohn-Luttinger analysis:

As before, consider Hubbard U

To first order in U, $g_4=g_3=U$, and we only have a repulsive s-wave component $\Gamma_{a,0} < 0$, $\Gamma_{b,0} = 0$

To order U²
$$\Gamma_0 = \begin{pmatrix} k, \sigma & k', \sigma \\ & k, \sigma' & \cdots & -k', \sigma' \end{pmatrix} +$$

Inter-pocket repulsion g_3 exceeds intra-pocker repulsion g_4 , and $\Gamma_{b,0}$ becomes positive, i.e., the system is unstable towards a superconductivity with $\Delta = \Delta_b (1,-1)$.

> Agterberg, Barzykin, Gorkov, Mazin, Kuroki,

sign-changing s-wave gap (s⁺⁻)





Photoemission in 1111 and 122 FeAs



T. Kondo et al.



 $BaFe_2(As_{1-x}P_x)_2$



laser

ARPES

T. Shimojima et al

Almost angle-independent gap (consistent with s-wave)

Neutron scattering - resonance peak below 2D

s+- gap



Summary of Kohn-Luttinger physics:

At weak coupling, a fermionic system may undergo a superconducting instability, despite that the interaction is repulsive. The instability is never an ordinary s-wave

> d-wave $(d_x^2 - y^2)$ pairing in the cuprates d+id $(d_x^2 - y^2 + d_{xy})$ in doped graphene s+- in Fe-pnictides

This story is a little bit too good to be true.

In all three cases, we assumed that bare interaction is a Hubbard U, in which case, in a relevant channel $\Gamma = 0$ to order U and becomes positive (attractive) to order U²

In reality, to order U, $\Gamma = -U_{small} + U_{large}$ small (large) is a momentum transfer

For any realistic interaction, $U_{small} > U_{large}$

Then bare Γ <0, and the second order term has to overcome it

Houston, we have a problem



One possibility is to abandon weak coupling (next lecture – spin fluctuation induced pairing)

Another is to keep couplings as weak, but see whether we can additionally enhance KL terms (this is what we will do now)

The idea is that, if superconductivity competes with other potential instabilities, like SDW or CDW, there may be additional enhancement of the pairing interaction at large momentum transfer, and simultaneous reduction (and even sign change) of the pairing interaction at a small momentum transfer



Consider Fe-pnictides as an example

 g_3 and g_4 are bare interactions, at energies of a bandwidth

For SC we need interactions at energies smaller than the Fermi energy



Couplings flow due to renormalizations in particle-particle and particle-hole channels

Suppose that hole and electron pockets are identical

$$\varepsilon_k^h = -\varepsilon_{k+Q}^e$$

Renormalizations in particle-particle and particle-hole channels are both logarithmically singular

particle-particle channel – Cooper logarithm particle-hole cannel – logarithm due to nesting



Then we have to treat particle-particle (SC) and particle-hole channels on equal footings Introduce all relevant couplings between low-energy fermions

With apologies, I will label interactions as u instead of g



Intra-pocket repulsion

Inter-pocket repulsion

Inter-pocket forward and backward scattering

We need enhancement of u_3 relative to u_4 for superconductivity

Renormalization of u₃



Kohn-Luttinger diagrams, "nesting logarithms"

Renormalization of u₁



Also contains "nesting logaritms"

$$\dot{u}_1 = u_1^2 + u_3^2$$

$$\dot{u}_2 = 2u_2(u_1 - u_2)$$

$$\dot{u}_3 = u_3(4u_1 - 2u_2 - 2u_4)$$

$$\dot{u}_4 = -u_3^2 - u_4^2$$

One-loop parquet RG





One-loop parquet RG



The fixed point: the pair hopping term us is the largest

$$u_1 = -u_4 = \frac{|u_3|}{\sqrt{5}}, u_2 \propto |u_3|^{1/3}$$

Over-screening: intraband interaction u_4 changes sign and becomes attractive below some scale.

We can re-write parquet RG equations as equations for density-wave and superconducting vertices







At some scale, generated by the system, s+- SC vertex changes sign and becomes attractive

Lower boundary for parquet RG is the Fermi energy, E_F

Below E_F – decoupling between SDW and SC channels

$$\frac{d\Gamma_j}{dL} = \Gamma_j^2$$

Boundary values:
$$u_i (E \sim E_F) = u_i^R$$

 $\Gamma_{SDW} = u_1^R + u_3^R$, $\Gamma_{SC} = u_3^R - u_4^R$

Whichever vertex is the larger by magnitude at E_F, wins



0

0

0.02

0.04

0.06

х

0.08

E

0.10 0.12

Perfect nesting – SDW wins

Non-perfect nesting –SDW vertex remains the strongest, but the SDW instability is cut, and s⁺⁻ SC wins

It is essential that Γ_{SC} is already attractive

In real systems, there are 2-3 hole and 2 electron Fermi surfaces



SC vertex can overshoot SDW vertex, in which case SC becomes the leading instability

A very similar behavior in doped graphene



Because of van-Hove points

• superconducting susceptibility gets an extra boost:

$$\Pi_{\rm pp} (0) \propto \log^2 \frac{\Lambda}{T}$$

Because of nesting and van-Hove points

• density-wave susceptibilities at Q_i become equivalent to SC susceptibility

$$\Pi_{\rm ph} \left(Q_{\rm i} \right) \propto \log^2 \frac{\Lambda}{T}$$

Like before, we introduce all possible interactions between low-energy fermions

$$H_{two-particle} = \sum_{\alpha,\beta=1}^{3} \frac{g_1}{2} \psi_{\alpha}^{+} \psi_{\beta}^{+} \psi_{\alpha} \psi_{\beta} + \frac{g_2}{2} \psi_{\alpha}^{+} \psi_{\beta}^{+} \psi_{\beta} \psi_{\alpha} + \frac{g_3}{2} \psi_{\alpha}^{+} \psi_{\alpha}^{+} \psi_{\beta} \psi_{\beta} \psi_{\beta} + \sum_{\alpha=1}^{3} \frac{g_4}{2} \psi_{\alpha}^{+} \psi_{\alpha}^{+} \psi_{\alpha} \psi_{\alpha} \psi_{\alpha}$$



RG equations (perfect nesting)





all 3 patches are involved

General RG equations

$$y = \Pi_{\rm pp}(\mathbf{k} = 0, E) = \frac{\nu_0}{4} \ln^2 \frac{\Lambda}{E}$$



n=3 is the # of patches (**n=2** for the cuprates)



Inter-patch pairing interaction g₃ again becomes the largest one

SDW, CDW, and SC vertices









 $\neg d$ -wave

SC





 g_3

 g_4

$$\Delta_{j} = \Delta_{j}^{0} \left(1 - \Gamma_{j} \log^{2} \frac{\Lambda}{E} \right)$$



• The SDW vertex is the largest one at intermediate energies

- •Interaction with SDW channel pushes SC vertex up, and Γ^{d-wave}_{SC} changes sign and becomes attractive
- The superconducting vertex eventually takes over and becomes the leading instability at low energies

Functional RG – the same result Thomale et al



Conclusions:

The issue is the pairing by electron-electron interaction

I. Kohn-Luttinger mechanism:

For on-cite Hubbard interaction

p-wave pairing for isotropic dispersion d-wave (d_x^2, y^2) pairing in the cuprates d+id $(d_x^2, y^2 + d_{xy})$ in doped graphene s+- in Fe-pnictides

II. If first-order (bare) interaction in these channels is repulsive, SC is still possible when fluctuations in the density-wave channel are comparable to SC fluctuations (SC vertex is pushed up due to interaction with SDW)

THANK YOU