Pseudogap state of ultracold Fermi gases in the BCS-BEC crossover regime

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Outline of talk:

• Introduction: BCS-BEC crossover and pseudogap
• Model and formalism: Nozieres-Schmitt-Rink theory
• Pseudogap in a homogeneous Fermi gas: single-particle spectral weight and density of states above Tc, pseudogap temperature and phase diagram
• Summary 1
• Photoemission spectroscopy for a Fermi gas
• Pseudogap signature in photoemission spectra of a trapped Fermi gas
• Summary 2
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BCS-BEC crossover

strong-coupling  weak-coupling

BEC  BCS

Theory: Eagles, Leggett, Nozieres-Schmitt-Rink

$T_c$
BCS-BEC crossover in atomic Fermi gas

- **pair condensation**

\[ \frac{T_c}{T_F} \sim 0.08 - 0.2 \gg 10^{-4} - 10^{-2} \]

- **40K**

Regal et al. PRL (2004)

- **high-Tc superfluid!**

- **Feshbach resonances** allow one to control the interatomic interaction

\[ T_F = 0.35 \mu K \]
Feshbach resonance

- s-wave scattering length tunable by magnetic field

\[ a(B) = a_{bg} \left( 1 - \frac{w}{B - B_0} \right) \]

molecules form when \( a > 0 \)
Evolution of Tc in BCS-BEC crossover

- BCS transition temperature

\[ T_{\text{BCS}} = \frac{8\gamma}{\pi e^2} \varepsilon_F e^{-\frac{\pi}{2k_F a_s}} = \frac{\gamma}{\pi} \Delta_0 \]

\( \Delta_0 \) : gap at \( T=0 \)
(pair binding energy)

Cooper pair formation at \( T_{\text{BCS}} \)
Evolution of \( T_c \) in BCS-BEC crossover

\[ \lambda_{dB} = \left( \frac{2\pi \hbar^2}{mk_B T} \right)^{1/2} \propto \frac{1}{\sqrt{T}} \]

\( \lambda_{dB} \approx d \) (interatomic distance) at \( T = T_{BEC} \)
Size of pair shrinks as increasing the interaction condition for BEC is not satisfied at $T_{BCS}$: $\lambda_{dB} < d$
necessary to lower $T$ to achieve $\lambda_{dB} \simeq d$
Note that pair formation and condensation occurs at $T_{BCS}$ simultaneously because of large overlapping pairs
Pseudogap in high-Tc cuprates

- Pseudogap observed in ARPES, tunneling, NMR, etc.

- Origin of pseudogap
  - incoherent preformed pairs
  - strong AF spin fluctuations
  - hidden order etc.

- Theory
  Yanase, Randeria, Strinati, Varma, Metzner ...

- Bi$_2$Sr$_2$CaCuO$_{8+\delta}$

- Renner et al. PRL (1998)

- Origin of pseudogap
  - AFM
  - PG
  - SC

- Temperature (K)
  $T^*$
  $T > T_c$
  $T < T_c$
**Pseudogap in atomic Fermi gases**

- $T_{BCS} \sim \text{pair formation temperature}$

- **Pseudogap** is considered to exist in the temperature region $T_c \lesssim T \lesssim T_{BCS}$ due to the presence of incoherent non-condensed pairs.
We calculate the density of states and spectral weight including strong coupling effects associated with pairing fluctuations to directly identify the pseudogap.

Useful to clarify the possibility of preformed pair scenario for the pseudogap of high-Tc cuprates.
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Model

- Two-component Fermi gas: pseudospin \( \sigma = \uparrow, \downarrow \)
- Single-channel model

\[
V(r) = -U \delta(r) \quad (U > 0)
\]

\[
H - \mu N = \sum_{p, \sigma} (\varepsilon_k - \mu) c^\dagger_{p \sigma} c_{p \sigma} - U \sum_q \sum_{p, p'} c^\dagger_{p + \frac{q}{2} \uparrow} c^\dagger_{-p + \frac{q}{2} \downarrow} c_{-p' + \frac{q}{2} \downarrow} c_{p' + \frac{q}{2} \uparrow}
\]

- s-wave scattering length \( a_s \) tunable by Feshbach resonance

\[
\frac{4\pi a_s}{m} = \frac{-U}{1 - U \sum_p \frac{1}{2\varepsilon_p}}
\]
BCS theory implicitly assumes that all the Cooper pairs are Bose condensed in the same \( q=0 \) state. Cooper pairs with finite \( q \) are ignored. (\( q \) center of mass momentum)

In the BEC region \( (a_s > 0) \), pairs become stable two-particle bound states which can occupy finite momentum states. As \( T \) increases, more and more pairs leave the condensate. BCS theory fails to describe these situations.

NSR theory includes effects of pairs outside the condensate with \( q>0 \) involved in the pairing fluctuation diagrams.

\( T_c \) and \( \mu \) are determined in a self-consistent manner by solving the coupled equations of Thouless criterion and number equation. \( \mu = \varepsilon_F \) in the BCS theory.
\( T_c : \) Thouless criterion

Many-body \( T \)-matrix

\[ \Gamma(q, i\nu_n) = \frac{-U}{1 - U\Pi(q, i\nu_n)} \]

\[ \Pi(q, i\nu_n) = T \sum_{p,\omega_n} G^0_{p+q/2}(i\nu_n + i\omega_n)G^0_{-p+q/2}(-i\omega_n) \]

pairing fluctuations

\[ \Gamma(q = 0, \omega = 0)^{-1} = 0 \]

at \( T = T_c \)  \( \text{Thouless criterion} \)

\[ 1 = -\frac{4\pi a_s}{m} \sum_p \left[ \frac{1}{2(\varepsilon_p - \mu)} \tanh \frac{\beta(\varepsilon_p - \mu)}{2} - \frac{1}{2\varepsilon_p} \right] \]  \( \text{BCS gap equation} \)
\[ \mu : \text{number equation} \]

\[ N = -\frac{\partial \Omega}{\partial \mu} \quad \Omega = \Omega_0 + \delta \Omega \quad \Omega_0 : \text{free Fermion} \]

Correction from pairing fluctuations (left out in BCS)

\[ \delta \Omega = \quad \quad \quad + \quad \quad + \quad \quad + \ldots \]

\[ N = N_{F0} + 2N_B \]

\[ = N_{F0} - T \frac{\partial}{\partial \mu} \sum_{q, \nu_n} e^{i\delta \nu_n} \log \left[ 1 + \frac{4\pi a_s}{m} \left( \Pi(q, i\nu_n) - \sum_p \frac{1}{2\varepsilon_p} \right) \right] \]

\[ N_B : \text{number of pairs with } q>0 \]
**Thouless criterion (Gap equation)**

\[
1 = -\frac{4\pi a_s}{m} \sum_p \left[ \frac{1}{2(\varepsilon_p - \mu)} \tanh \frac{\beta(\varepsilon_p - \mu)}{2} - \frac{1}{2\varepsilon_p} \right]
\]

**Number equation**

\[
N = N_{F0} - T \frac{\partial}{\partial \mu} \sum_{q,\nu_n} e^{i\delta\nu_n} \log \left[ 1 + \frac{4\pi a_s}{m} \left( \Pi(q,\nu_n) - \sum_p \frac{1}{2\varepsilon_p} \right) \right]
\]

- **BCS limit** \(1/k_Fa_s \to -\infty\)

**Number equation**

\[
\mu = \varepsilon_F
\]

**Gap equation**

\[
T_c = \frac{8\gamma}{\pi e^2 \varepsilon_F} e^{\frac{\pi}{2 k_F a_s}} = T_{BCS}
\]
**Thouless criterion (Gap equation)**

\[
1 = -\frac{4\pi a_s}{m} \sum_p \left[ \frac{1}{2(\varepsilon_p - \mu)} \tanh \frac{\beta(\varepsilon_p - \mu)}{2} - \frac{1}{2\varepsilon_p} \right]
\]

**Number equation**

\[
N = N_{F0} - T \frac{\partial}{\partial \mu} \sum_{q, \nu_n} e^{i\delta \nu_n} \log \left[ 1 + \frac{4\pi a_s}{m} \left( \Pi(q, i\nu_n) - \sum_p \frac{1}{2\varepsilon_p} \right) \right]
\]

**BEC limit**

\[
\frac{1}{k_F a_s} \to \infty
\]

\[
\mu = -\frac{1}{2ma_s^2}
\]

\[
N = 2 \sum_q n_B(\varepsilon_q - \mu_B)
\]

\[
\mu_B = 2\mu + \frac{1}{ma_s^2}
\]

\[
E_{\text{bind}} = \frac{1}{ma_s^2}
\]

**ideal Bose gas of N/2 bosons**

\[
T_c = T_{\text{BEC}} = 0.218T_F
\]

**molecular binding energy**
Tc and $\mu_c$ in NSR theory

- Tc and $\mu(T_c)$ exhibit smooth crossover from the BCS region to the BEC region

- $\mu_c < 0$ in the BEC side

stable molecular bound state $\left(\frac{1}{k_Fa_s}\right)^{-1} \gtrsim 0.35$
Single-particle Green’s function in T-matrix app.

- Single-particle Green’s function

\[
G_p(i\omega_n) = \frac{1}{i\omega_n - (\varepsilon_p - \mu) - \Sigma_p(i\omega_n)}
\]

Number equation

\[
N = 2T \sum_{p,\omega_n} G_p(i\omega_n)e^{i\omega_n\delta}
\]

Self-energy

\[
\Sigma_p(i\omega_n) = T \sum_{q,\nu_n} \Gamma(q, i\nu_n) G_{q-p}^0(i\nu_n - i\omega_n)
\]

- Self-energy couples the pairing fluctuations into the single-particle spectrum.

- Density of states

\[
\rho(\omega) = -\frac{1}{\pi} \sum_p \text{Im} G_p(i\omega_n \rightarrow \omega^+)
\]

- Spectral weight

\[
A_p(\omega) = -\frac{1}{\pi} \text{Im} G_p(i\omega_n \rightarrow \omega^+).
\]
Destroying an atom involves destroying an excitation and at the same time creating one. This is the source of the negative energy pole of the SW.

\[ E_p = \sqrt{(\varepsilon_p - \mu)^2 + \Delta^2} \]

\[ A_p^{BCS}(\omega) = u_p^2 \delta(\omega - E_p) + v_p^2 \delta(\omega + E_p) \]

\[ \rho(\omega) = \sum_p A_p(\omega) \]

\[ \rho^{BCS}(\omega) \]

\[ \rho^0(\omega) \]

\[ c_{p\uparrow} = u_p \gamma_{p\uparrow} + v_p \gamma_{-p\downarrow} \]
Density of states at $T_c$

- **BCS side** ($a_s < 0$)
- **BEC side** ($a_s > 0$)

Suppression of DOS near the Fermi level = Pseudogap

- Pseudogap is most remarkable at the unitarity limit and disappears in both the BCS and BEC limits.
Spectral weight at \( T_c \)

**BCS**

\[(k_Fa_s)^{-1} = -0.6\]

**Unitarity**

\[(k_Fa_s)^{-1} = 0.01\]

**BEC**

\[(k_Fa_s)^{-1} = 0.6\]

- Double-peak structure (Levin, Strinati)
  - \( \omega_{peak} = \pm \sqrt{(\epsilon_p - \mu)^2 + \Delta_{pg}} \)
  - \( \Delta_{pg} \): pseudogap
  - similar to BCS SW

- Double-peak structure in SW yields the pseudogap in DOS

\[
A_p(BCS)(\omega) = u_p^2 \delta(\omega - E_p) + v_p^2 \delta(\omega + E_p)
\]

\[
E_p = \sqrt{(\epsilon_p - \mu)^2 + \Delta^2}
\]
Simple picture for origin of pseudogap

- BCS Green’s function

\[
G_{11}(p, i\omega_n) = \frac{u_p^2}{i\omega_n - E_p} + \frac{v_p^2}{i\omega_n + E_p}
\]

\[
= \frac{1}{(i\omega_n - \xi_p)} - \frac{\Delta^2}{i\omega_n + \xi_p}
\]

\[G^0_{-p}(-i\omega_n)\] : hole Green’s func.

- \(\Gamma_{q=0}(i\nu_n = 0)\) diverges at \(T_c\) (Thouless criterion)

\[
\Sigma_p(i\omega_n) = T \sum_{q,\nu_n} \Gamma_q(i\nu_n) G^0_{q-p}(i\nu_n - i\omega_n)
\]

\[\simeq T \sum_{q,\nu_n} \Gamma_q(i\nu_n) \times G^0_{-p}(-i\omega_n)\]

\[\Delta^2_{pg} = -T \sum_{q,\nu_n} \Gamma_q(i\nu_n)\]

pseudogap describes particle-hole coupling strength
Spectral weight at $T_c$

**BCS**

$$(k_F a_s)^{-1} = -0.6$$

**Unitarity**

$$(k_F a_s)^{-1} = 0.01$$

**BEC**

$$(k_F a_s)^{-1} = 0.6$$

- $\Delta_{pg}$ evolves as increasing interaction strength
- Broadened peaks indicate short life time of quasiparticles

$$\rho(\omega) = \sum_{p} A_p(\omega)$$
Spectral weight at $T_c$

**BCS** \( (k_F a_s)^{-1} = -0.6 \)

**Unitarity** \( (k_F a_s)^{-1} = 0.01 \)

**BEC** \( (k_F a_s)^{-1} = 0.6 \)

- **asymmetric** upper and lower peaks
- **sharp coherent upper peak**
- **broad incoherent lower peak**

atoms from dissociated molecules

hole-type excitation: many-body effect
(completely absent in the BEC limit)
Pseudogap in DOS disappears at $T^*$, while the double peaks in SW merge into a single peak at $T^{**}$.

$T^* \approx 1.14 T_c$

$T^{**} \approx 1.03 T_c$

$(k_F a_s)^{-1} = -0.6$
Density of states above $T_c$ (BCS side)

- Pseudogap in DOS persists to higher temperatures than the double-peak structure.
  - $T^* > T^{**}$
- Pseudogap arises from broad suppressed single peak
Density of states at above $T_c$ (BEC side)

$$(k_F a_s)^{-1} = 0.4$$

$T^* \approx 1.53 T_c$

- $T^* \neq T^{**}$
- Disappearance of double-peak structure at very high temperatures: $T^{**} \gtrsim \varepsilon_F$
Density of states at above \( T_c \) (BEC side)

\[(k_F a_s)^{-1} = 0.4\]

- The double-peak structure persists to higher temperatures than the pseudogap.
- \( T^* < T^{**} \)

- Lower broad peak is smeared out in density of states.
Physical backgrounds of T* and T**

- Double peaks merge into a single broad peak at $T^{**}$.

\[ \Delta_{pg} \sim \text{Im}\Sigma(p_F, \omega \approx 0) \]

**BCS-type quasiparticles** are not well-defined above $T^{**}$, because of their short life time.

- Pseudogap in DOS disappears at $T^*$.

Suppression of DOS around Fermi level indicates that fermionic degrees of freedom are transformed into bosonic ones.

Pairs are formed below $T^*$

- $T^* \neq T^{**}$ suggests that formation of **pairs** and **BCS-type quasiparticles** do **not** occur at the same temperature. (In the BCS theory, they both occur at $T_c$.)
Phase diagram of the BCS-BEC crossover

- $T^*$: pseudogap in DOS
- $T^{**}$: double-peak structure in SW
- $E_{\text{bind}}$: molecular binding energy $E_{\text{bind}} = 2|\mu|$
Since the pseudogap is a crossover phenomenon, the pseudogap temperature may depend on what we measure. $T^*$: DOS $T^{**}$: SW
Summary: part 1

- We investigated the pseudogap phenomenon of a Fermi gas in the BCS-BEC crossover within the many-body T-matrix theory (NSR theory).
- We calculated the DOS and SW above Tc, and demonstrated that pseudogap indeed appears in these quantities in the BCS-BEC crossover region.
- In the BCS side ($a_s < 0$), the pseudogap persists to higher temperatures than the double-peak structure in the spectral weight. ($T^* > T^{**}$)
- In the BEC side ($a_s > 0$), the double-peak structure persists to higher temperatures than the pseudogap. ($T^* < T^{**}$)
- We have determined the pseudogap region in the BCS-BEC phase diagram.
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Photoemission spectroscopy

- Powerful technique to probe occupied single-particle states

ARPES for high-Tc cuprates

- Direct measurements of spectral weight $A(p, \omega)$
- Useful for determining quasiparticle spectrum, symmetry of order parameter etc.

Matsui et al., PRL (2003)
Photoemission spectroscopy for atomic gases

- Photoemission spectroscopy for Fermi gases in the BCS-BEC crossover  D. Jin’s group (JILA)

- Applied radio-frequency pulse transfers atoms to a third empty atomic state (no final state interaction for $^{40}$K)

\[ |3\rangle \xrightarrow{\hbar \nu} |\rangle \]

involved in pairing

\[ |2\rangle \leftrightarrow |1\rangle \]

- Momentum-resolved rf current of atoms in the third state

\[ I(p, \Omega) \propto A(p, \xi_p - \Omega) f(\xi_p - \Omega) \]

\[ \Omega = h \nu - \phi : \text{rf detuning} \]

\[ A(p, \omega) = -\frac{1}{\pi} \text{Im} G_p(\omega^+) \]
Tc and $\mu$ of trapped Fermi gases

- effects of trapping potential

\[ \mu \rightarrow \mu - V(r) = \mu(r) \]

Local density approximation

\[ \varepsilon_F = (3N)^{1/3} \omega_{tr} \]

\[ V(r) = m\omega_{tr}^2 r^2 / 2 \]

\[ G_p(i\omega_n, r) = \frac{1}{i\omega_n - (\varepsilon_p - \mu(r)) - \Sigma_p(i\omega_n, r)} \]

Spatial dependence

\[ A(p, \omega, r) \rho(\omega, r) \]
Local DOS: **unitarity limit**

\[
R_F = \sqrt{\frac{2\varepsilon_F}{m\omega^2}} : \text{T-F radius}
\]

- Pseudogap disappears from the **outer region** of the cloud, because **low particle density** suppresses pair fluctuations.
The pseudogap temperature is defined at $r = 0$. 

\[
T^* \approx 1.07T_c
\]
Local SW : unitarity limit

- $A(p, \omega, r) \in F$
- $T = T_c$
- $1.20T_c \approx T^{**}$
- $1.65T_c$

- Increasing $r$ and $T$ give similar effects: $\mu(r) \downarrow$

$r \uparrow$

or

$T \uparrow$
Density distribution of pairs

\[ n_F(r) = 2T \sum_{\mathbf{p}, \omega_n} G^0_{\mathbf{p}}(i\omega_n, r) e^{i\omega_n \delta} \]

\[ n_B(r) = T \sum_{\mathbf{p}, \omega_n} \left[ G_{\mathbf{p}}(i\omega_n, r) - G^0_{\mathbf{p}}(i\omega_n, r) \right] e^{i\omega_n \delta} \]
Phase diagram of a trapped Fermi gas

$T^*$: pseudogap in DOS

$T^{**}$: double-peak structure in SW

$E_{\text{bind}}$: molecular binding energy $E_{\text{bind}} = 2|\mu|$
Calculation of photoemission spectrum

- rf-pulse is applied to the whole gas cloud
- observed spectrum involves contributions from all spatial regions of the cloud.

\[
I_{\text{ave}}(\mathbf{p}, \Omega) = \frac{1}{V} \int d\mathbf{r} I(\mathbf{p}, \Omega, r)
\]

\[
I(\mathbf{p}, \Omega, r) = 2\pi t_F^2 A(\mathbf{p}, \xi_p(r) - \Omega, r) f(\xi_p(r) - \Omega)
\]

- momentum-resolved rf current

- averaged occupied SW and DOS

\[
\overline{A(\mathbf{p}, \omega)f(\omega)} = \frac{I_{\text{ave}}(\mathbf{p}, \Omega \rightarrow \xi_p - \omega)}{(2\pi t_F^2)}
\]

\[
\overline{\rho(\omega)f(\omega)} = \sum_{\mathbf{p}} \frac{I_{\text{ave}}(\mathbf{p}, \Omega \rightarrow \xi_p - \omega)}{(2\pi t_F^2)}
\]

- homogeneous gas

\[
A(\mathbf{p}, \omega)f(\omega) = \frac{I(\mathbf{p}, \Omega \rightarrow \xi_p - \omega)}{(2\pi t_F^2)}
\]

\[ \frac{(\omega + \mu)}{\varepsilon_F} = \frac{1}{(k_F a_s)^{-1}} \]

\[ (k_F a_s)^{-1} = -1 \]

\[ (k_F a_s)^{-1} = 0 \]

\[ (k_F a_s)^{-1} = 1 \]


**BCS regime**

**unitarity**

**BEC regime**

\[ p^2 A(p, \omega) f(\omega) \]
Averaged spectra have both the features of the pseudogapped spectrum in the center and the single particle spectrum at the edge.
Spatially averaged density of states

Theory curves agree well with the photoemission data of the Jin’s group.
Observation of pseudogap

\[ (k_F a_s)^{-1} \approx 0.15 \]


back-bending peak
= pseudogap!
Photoemission spectra above $T_c$

$(k_F a_s)^{-1} = 0.2$

$(\omega + \mu)/\varepsilon_F$

$T = T_c$

$T/T_c = 1.28$

$T/T_c = 1.84$

$(k_F a_s)^{-1} \approx 0.15$

$p^2 A(p, \omega) f(\omega)$

$T/T_c = 0.74$

$(T/T_c)_0 = 0.13$

$= 1.24$

$= 0.21$

$= 1.47$

$= 0.25$

$= 2.06$

$= 0.35$
Photoemission spectra above $T_c$

$(k_F a_s)^{-1} = 0.2$

- The back-bending peak disappears at $T^{**}$ reflecting the disappearance of the pseudogap in the trap center.

- The lower broad peak remaining at high temperatures is related to the universal behavior of Fermi gas with contact interaction (nothing to do with the pseudogap physics).

Tan (2008), Randeria (2010)
• We calculated the photoemission spectrum of a trapped Fermi gas above Tc by including pairing fluctuations within the T-matrix approximation, as well as effects of a trap potential within the LDA.
• We showed that spatially inhomogeneous pair fluctuations produced by the trap potential is crucial to understand the observed photoemission spectrum.
• The quantitative agreement with the experimental data strongly supports that our theoretical approach correctly describes the pseudogap phenomena in a cold Fermi gas.
Photoemission spectra above $T_c$

$$p^2 A(p, \omega) f(\omega)$$