Polarised Fermi gases within the T-matrix approach

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Outline

- introduction
- Nozières-Schmitt-Rink (NSR) approach and its breakdown
- $T = 0$: particle-particle RPA
- $T > 0$: self-consistent treatment of "mean-field" shift
- summary and outlook

References

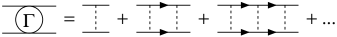
- M. U. and P. Schuck, PRA 90, 023632 (2014)
- P.-A. Pantel, D. Davesne, and M. U., PRA 90, 053629 (2014); erratum PRA 94, 019901 (2016)

Introduction

- BCS-BEC crossover for two-component ($\sigma = \uparrow, \downarrow$) Fermi gases can be studied with ultracold atoms (e.g. ^{6}Li) with a Feshbach resonance
- BCS mean-field strongly overestimates T_c (does not tend towards the correct BEC limit)
- T-matrix approaches (NSR and variants) are very common to describe the crossover
- what happens at finite polarisation $P = \dfrac{\rho_\uparrow - \rho_\downarrow}{\rho_\uparrow + \rho_\downarrow}$?
- exotic forms of pairing (LOFF) ?
- at low T, experiment for the unitary gas shows 1st order phase transition (phase separation between normal and superfluid phases)
- special case: limit $P \to 1$ (single spin $\downarrow$ atom in a bath of spin $\uparrow$ atoms): polaron + Fermi sea or molecule + Fermi sea ?
- polaron also well described by T-matrix (equivalent to Chevy ansatz, cf. Combescot et al., PRL 98)
- problem: NSR approach fails in the polarised case!

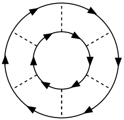
Original Nozières-Schmitt-Rink approach

[Nozières and Schmitt-Rink, JLTP 59, 195 (1985), Sá de Melo et al., PRL 71, 3202 (1993)]



- ladder approximation for T-matrix Γ
- T_c as function of μ: Thouless criterion

$$\Gamma^{-1}(\omega = 0, k = 0) = 0$$

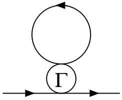


$\rightarrow$ $T_c(\mu)$ is the same as in BCS

- density from thermodynamic potential

$\Leftrightarrow$ truncate Dyson equation at first order:

$$G = G_0 + G_0^2 \Sigma \qquad (\Sigma = \text{self-energy})$$



- density $\rho = \rho_0 + \rho_1$

$$\rho_1 = \frac{\partial}{\partial \mu} \int \frac{d^3k}{(2\pi)^3} \int \frac{d\omega}{2\pi} \, g(\omega) \, \delta(\omega, k)$$

(g = Bose function, $\delta = \text{Im} \log(-\Gamma)$ = in-medium scattering phase shift)

$\rightarrow$ ρ_1 includes density of correlated pairs above T_c

$\rightarrow$ $T_c(\rho)$ interpolates between BCS and BEC limits

Breakdown of the NSR approach in the polarised case

- generalise the NSR approach to the case $\delta\mu = \mu_\uparrow - \mu_\downarrow \neq 0 \qquad (\bar{\mu} = \frac{\mu_\uparrow + \mu_\downarrow}{2})$
- Thouless criterion for T_c has to be changed to

$$\exists k : \quad \Gamma^{-1}(\omega = 0, k) = 0$$

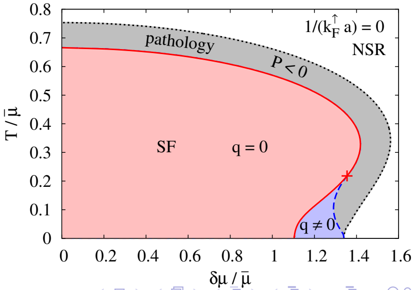
  if pole appears first for $\vec{k} \neq 0 \;\; \rightarrow$ transition towards LOFF phase
- the correction to the density of each spin state σ is given by

$$\rho_{1\sigma} = \frac{\partial}{\partial \mu_\sigma} \int \frac{d^3k}{(2\pi)^3} \int \frac{d\omega}{2\pi} g(\omega)\, \delta(\omega, \vec{k})$$

- problem: near unitarity sometimes $P < 0$ for $\delta\mu > 0$

  [Liu, Hu (2006); Parish et al. (2007)]
- even in the unpolarised case: spin susceptibility $\chi = \frac{\partial(\rho_\uparrow - \rho_\downarrow)}{\partial \delta\mu}$ has the wrong sign

  [Kashimura et al. (2012)]



$T = 0$: particle-particle RPA (pp-RPA) vs. NSR approach

- consider first the case $T = 0$
  $\rightarrow$ system in the normal phase only beyond some critical polarisation P_c
- ladder approximation = particle-particle RPA

pp-RPA	NSR
$T = 0$ formalism	Matsubara formalism
$G_{0\sigma}(\omega, p) = \frac{\theta(k_F^\sigma - p)}{\omega - \epsilon_p - i\eta} + \frac{\theta(p - k_F^\sigma)}{\omega - \epsilon_p + i\eta}$	$G_{0\sigma}(i\omega_n, p) = \frac{1}{i\omega_n - \epsilon_p + \mu_\sigma}$
k_F^σ fixed	μ_σ fixed
$\mu_\sigma = \epsilon_F^\sigma + \mu_{1\sigma}$	$\rho_\sigma = \rho_{0\sigma} + \rho_{1\sigma}$
$\mu_{1\sigma} = \partial\mathcal{E}_1/\partial\rho_\sigma$	$\rho_{1\sigma} = -\partial\Omega_1/\partial\rho_\sigma$

- in perturbation theory, $T \rightarrow 0$ limit of Matsubara formalism and $T = 0$ formalism are equivalent [e.g., Dickhoff-Van Neck], but not necessarily in a non-perturbative approach

T matrix at $T = 0$

- free 2-particle (hole-hole + particle-particle) propagator: $J = J_{\text{hh}} + J_{\text{pp}}$

$$J_{\text{hh}}(\omega, \vec{k}) = -\int \frac{d^3p}{(2\pi)^3} \frac{\theta(k_F^{\uparrow} - p)\theta(k_F^{\downarrow} - |\vec{k} - \vec{p}|)}{\omega - \epsilon_{\vec{p}} - \epsilon_{\vec{k}-\vec{p}} - i\eta}\,, \quad J_{\text{pp}}(\omega, \vec{k}) = \int \frac{d^3p}{(2\pi)^3} \frac{\theta(p - k_F^{\uparrow})\theta(|\vec{k} - \vec{p}| - k_F^{\downarrow})}{\omega - \epsilon_{\vec{p}} - \epsilon_{\vec{k}-\vec{p}} + i\eta}$$

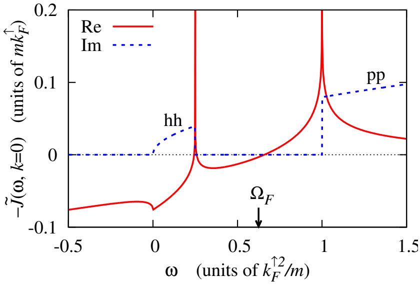
- T-matrix: $\Gamma = \dfrac{1}{\frac{1}{g} - J} = \dfrac{1}{\frac{m}{4\pi a} - \tilde{J}}$

- for small k, Γ has always poles!
  (in the gap between the hh and pp continua)

- critical polarisation P_c:
  Thouless criterion

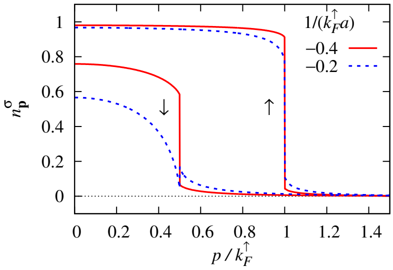
$$\exists k \;:\quad \Gamma^{-1}(\Omega_F, k) = 0$$

where $\Omega_F = \epsilon_F^{\uparrow} + \epsilon_F^{\downarrow}$



Occupation numbers at $T = 0$

- occupation numbers: $n_p^\sigma = -i \int \frac{d\omega}{2\pi} e^{i\omega\eta} G^\sigma(\omega, p)$
- as in NSR: $G = G_0 + G_0^2 \Sigma$
- example: $k_F^\downarrow = k_F^\uparrow/2$ ($P \approx 0.78$)
- for strong interaction, the jump of $n_p^\downarrow$ at $k_F^\downarrow$ becomes negative close to P_c (sometimes even $n_p^\downarrow < 0$ below $k_F^\downarrow$)



- problem of the truncation of the Dyson series at first order in Σ:

$\rightarrow$ jump $\quad n^\sigma_{p\to k^\sigma_{F-}} - n^\sigma_{p\to k^\sigma_{F+}} = 1 + \frac{d}{d\omega}\Sigma^\sigma(\omega, k_F^\sigma)\Big|_{\omega=\epsilon_F^\sigma}$

instead of $Z^\sigma_{k_F^\sigma}$ with $\quad Z_p^\sigma = \left(1 - \frac{d}{d\omega}\Sigma^\sigma(\omega, p)\Big|_{\omega=\epsilon_p^{\sigma *}}\right)^{-1}$

(where $\epsilon_p^{\sigma *} = \epsilon_p^\sigma + \Sigma^\sigma(\epsilon_p^{\sigma *}, p)$)

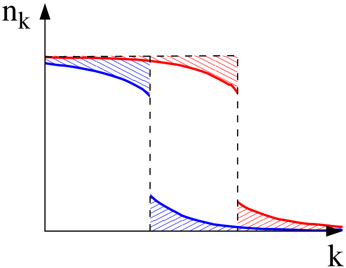
Luttinger theorem

- Luttinger theorem: $\rho_\sigma = \frac{k_F^{\sigma\,3}}{6\pi^2} = \rho_{0\sigma}$

  $\rightarrow \quad \rho_{1\sigma} = \int \frac{d^3k}{(2\pi)^3} n^\sigma_{1\,k} = 0$

  $\rightarrow$  $=$  and  $=$ 

  (weighted with k^2)



- satisfied in pp-RPA
- furthermore one can show:  $=$ 

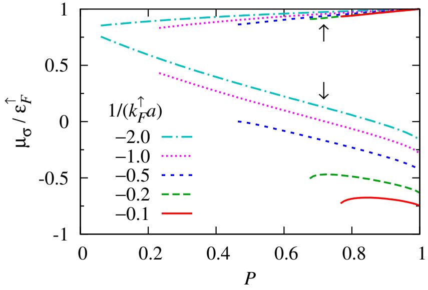
  numbers of particles scattered out of their Fermi sea are equal for both spins
- intuitively clear: $\uparrow$ and $\downarrow$ particles always scatter pairwise
- this explains why $n_k^\downarrow$ is much more strongly modified than $n_k^\uparrow$

Chemical potentials and polaron energy

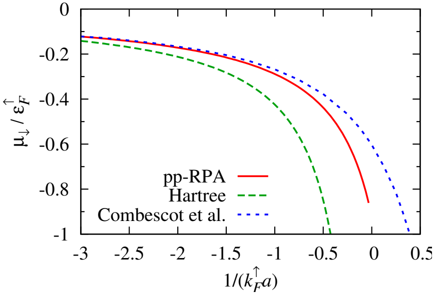
- NSR: μ is fixed, ρ is changed $\leftrightarrow$ here: ρ is fixed, μ is changed

$$\mu_\sigma = \frac{\partial \mathcal{E}}{\partial \rho_\sigma}\,, \qquad \mathcal{E} = \mathcal{E}_0 + \mathcal{E}_1\,, \qquad \mathcal{E}_1 = -\int \frac{d^3k}{(2\pi)^3} \int_{-\infty}^{\Omega_F} \frac{d\omega}{\pi}\, \mathrm{Im}\,\log\left(-\Gamma(\omega,k)\right)$$

μ_σ vs. polarisation P:



$\mu_\downarrow$ for $P \to 1$ (polaron):

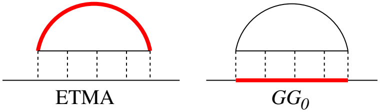


Combescot et al.: PRL 98, 180402 (2007)

Hartree: $\mu_\downarrow = (4\pi a/m)\rho_\uparrow$

Back to $T > 0$: alternative T-matrix approaches

- there are extensions of the NSR scheme that avoid the problem in the polarised case by dressing propagators in Σ, e.g.:
  - ETMA [Kashimura et al., PRA 86 (2012)]
  - GG_0 scheme [Chen et al., PRB 75 (2007)]



- here: generalise an approach by Zimmermann and Stolz (ZS) [Phys. Status Solidi B 131 (1985)] to the polarised case

- this approach has been used to describe the crossover from a BEC of deuterons to BCS pairing in low-density nuclear matter
  [Schmitt et al., Ann. Phys. (N.Y.) 202 (1990);
  Stein et al., Z. Phys. A 351 (1995);
  Jin et al., Phys. Rev. C 82 (2010)]

ZS approach for $T > 0$: a step towards self-consistency

- idea: self-consistent inclusion of shift of quasiparticle energy $\xi^*_{p\sigma}$

$$G_{0\sigma}(\omega, p) \to G^*_\sigma(\omega, p) = \frac{1}{\omega - \xi^*_{p\sigma}}\,, \qquad \xi^*_{p\sigma} = \epsilon_{p\sigma} - \mu_\sigma + \Sigma_\sigma(\xi^*_{p\sigma}, p)$$

- truncate Dyson series for correlations but not for the "mean field" shift

$$G_\sigma = G^*_\sigma + G^{*\,2}_\sigma(\Sigma_\sigma(\omega, p) - \Sigma(\xi^*_\sigma))$$

- the density correction due to correlations is independent of the spin!

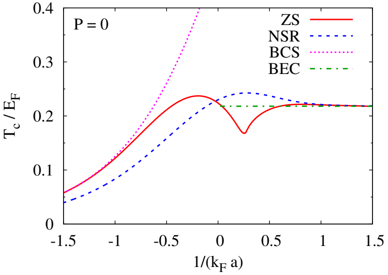
$$\rho_\sigma = \int \frac{d^3p}{(2\pi)^3} f(\xi^*_{p\sigma}) - \int \frac{d^3k}{(2\pi)^3} \int \frac{d\omega}{\pi} g'(\omega)\Big(\delta(\omega, k) - \frac{1}{2}\sin 2\delta(\omega, k)\Big)$$

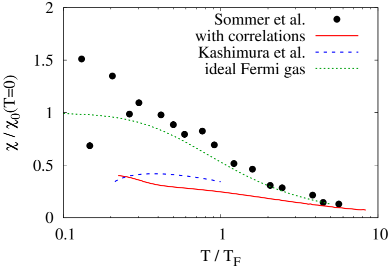
- additional approximation to simplify numerical implementation: constant shift U_σ calculated at the Fermi surface

$$\xi^*_{p\sigma} \approx \epsilon_p - \mu_\sigma + U_\sigma\,, \qquad U_\sigma = \mathrm{Re}\,\Sigma_\sigma(\xi^*_{k_F^\sigma\,\sigma}, k_F^\sigma)\,, \qquad \mu^*_\sigma = \mu_\sigma - U_\sigma$$

Unpolarised case: T_c and spin susceptibility

- T_c in the unpolarised case vs. $1/(k_F a)$
- both NSR and ZS schemes interpolate between BCS and BEC limits
- ZS approaches BCS limit much faster
- T_c too high on the BCS side
  $\rightarrow$ missing screening correction (GMB)
- ZS: unrealistic dip in T_c on the BEC side
- spin susceptibility at unitarity above T_c
  χ_0: ideal Fermi gas result
- $\chi > 0$: pathology of NSR cured in ZS
- $\chi < \chi_0$ seems plausible
  (pairs resist against polarisation)
- ZS results close to those of ETMA





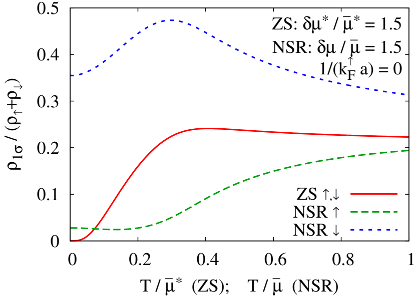
Polarised case: ZS and NSR density corrections

- back to finite polarisation
- for large enough $\delta\mu$, the normal phase extends down to $T = 0$
- study correction ρ_1 as a fct. of T
- within the ZS scheme, ρ_1 vanishes in the limit $T \to 0$

  $\longrightarrow$ Luttinger theorem!

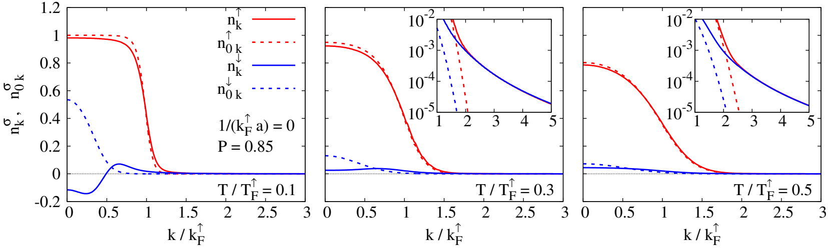
- within NSR, effects from mean-field shift and correlations are mixed

  $\longrightarrow$ $\rho_{1\uparrow}$ and $\rho_{1\downarrow}$ stay finite for $T \to 0$



Occupation numbers at $T > 0$

- occupation numbers $n_\uparrow(k)$ and $n_\downarrow(k)$ at $P = 0.85$ at different T



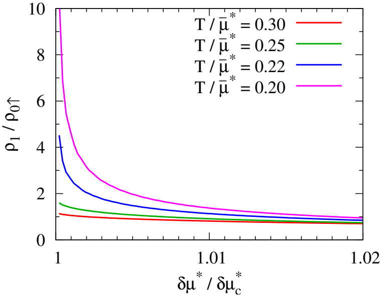
- near unitarity at large P and low T: same problem as in pp-RPA at $T = 0$ (because of truncation of Dyson series)

Problem: transition to the LOFF phase

- Thouless criterion for the phase boundary in the $T, \delta\mu^*$ plane:

$$\exists k \; : \quad \Gamma^{-1}(\omega = 0, k) = 0$$

- for given T_c, look for corresponding $\delta\mu_c^*$ (or vice versa)



- problem: density correction

$$\rho_1 = -\int \frac{d^3k}{(2\pi)^3} \int \frac{d\omega}{\pi} g'(\omega)\Big(\delta(\omega, k) - \frac{1}{2}\sin 2\delta(\omega, k)\Big)$$

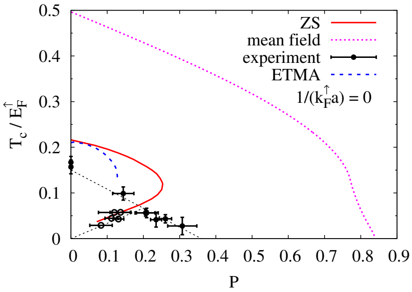
  diverges for $(T, \delta\mu^*) \to (T_c, \delta\mu_c^*)$ if the transition is towards the LOFF phase ($k \neq 0$)

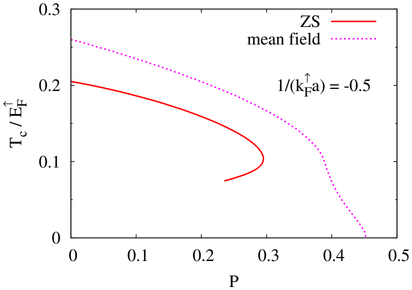
  $\rightarrow$ cannot describe transition at small T and finite P

- maybe not dramatic since this region is anyway thermodynamically unstable

Phase diagram

- ZS and BCS results for T_c vs. P
- experiment at unitarity [Shin et al., Nature 451 (2008)] shows 2nd-order phase transition at high T and phase separation (1st-order transition) at low T
- ZS significantly improved over BCS
- $\delta\mu > 0$ for $P > 0$ in the normal phase
- re-entrant behaviour beyond a point of $P_{\text{max}} \approx 0.25$
  qualitatively similar to ETMA where $P_{\text{max}} \approx 0.13$ [Kashimura (2012)]
- is the re-entrant behaviour related to the instability observed in experiment?





Summary

- NSR theory for the BCS-BEC crossover not applicable in the polarised case
- in the limit $T \to 0$, NSR does not coincide with $T = 0$ formalism (pp-RPA)
- nice features of pp-RPA at $T = 0$:
  - Luttinger theorem satisfied
  - reasonable description of the polaron (except very close to unitarity)
  - numbers of particles above the Fermi surface equal for both spins
- ZS approach for $T > 0$: self-consistent treatment of "mean-field" shift
  - the same correlated density ρ_1 for both spins
  - pathology of NSR approach is cured ($\rho_\uparrow > \rho_\downarrow$ for $\mu_\uparrow > \mu_\downarrow$)
  - reduces to pp-RPA in the limit $T \to 0$
  - cannot describe transition to LOFF phase
  - re-entrant behaviour at finite P and low T

Outlook

- first-order phase transition (phase separation):
  investigate thermodynamic stability in the region of re-entrant behaviour (matrix $\partial\mu_i/\partial\rho_j$ positive definite?)

- T_c (or P_c, respectively too high: screening corrections (GMB)

- RPA over-estimates correlations
  $\longrightarrow$ include correlated n_p^σ into Γ ("renormalised pp-RPA")

- resummation of Dyson series seems necessary close to unitarity
  but would probably destroy the nice properties of pp-RPA