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)
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 $P = \frac{\rho_\uparrow - \rho_\downarrow}{\rho_\uparrow + \rho_\downarrow}$

- 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 $\Gamma$
  \[
  \langle \Gamma \rangle = \cdots + \Gamma \cdots + \cdots \]

- $T_c$ as function of $\mu$: Thouless criterion
  \[
  \Gamma^{-1}(\omega = 0, k = 0) = 0
  \]
  \[\rightarrow T_c(\mu) \text{ is the same as in BCS}\]

- density from thermodynamic potential
  \[\iff\] truncate Dyson equation at first order:
  \[
  G = G_0 + G_0^2 \Sigma \quad (\Sigma = \text{self-energy})
  \]

- density $\rho = \rho_0 + \rho_1$
  \[
  \rho_1 = \frac{\partial}{\partial \mu} \int \frac{d^3k}{(2\pi)^3} \int \frac{d\omega}{2\pi} g(\omega) \delta(\omega, k)
  \]
  \[\text{(}g = \text{Bose function, } \delta = \text{Im log}(\Gamma) = \text{in-medium scattering phase shift)}\]
  \[\rightarrow \rho_1 \text{ includes density of correlated pairs above } T_c\]
  \[\rightarrow T_c(\rho) \text{ interpolates between BCS and BEC limits}\]
Breakdown of the NSR approach in the polarised case

- generalise the NSR approach to the case $\delta \mu = \mu^\uparrow - \mu^\downarrow \neq 0$ ($\bar{\mu} = \frac{\mu^\uparrow + \mu^\downarrow}{2}$)
- Thouless criterion for $T_c$ has to be changed to
  $$\exists k : \Gamma^{-1}(\omega = 0, k) = 0$$
  if pole appears first for $\vec{k} \neq 0 \rightarrow$ transition towards LOFF phase
- the correction to the density of each spin state $\sigma$ 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)]
Consider first the case $T = 0$ → system in the normal phase only beyond some critical polarisation $P_c$

Ladder approximation = particle-particle RPA

<table>
<thead>
<tr>
<th>pp-RPA</th>
<th>NSR</th>
</tr>
</thead>
<tbody>
<tr>
<td>$T = 0$ formalism</td>
<td>Matsubara formalism</td>
</tr>
<tr>
<td>$G_{0\sigma}(\omega, p) = \frac{\theta(k_F^\sigma - p)}{\omega - \epsilon_p - i\eta} + \frac{\theta(p - k_F^\sigma)}{\omega - \epsilon_p + i\eta}$</td>
<td>$G_{0\sigma}(i\omega_n, p) = \frac{1}{i\omega_n - \epsilon_p + \mu_\sigma}$</td>
</tr>
<tr>
<td>$k_F^\sigma$ fixed</td>
<td>$\mu_\sigma$ fixed</td>
</tr>
<tr>
<td>$\mu_\sigma = \epsilon_F^\sigma + \mu_{1\sigma}$</td>
<td>$\rho_\sigma = \rho_{0\sigma} + \rho_{1\sigma}$</td>
</tr>
<tr>
<td>$\mu_{1\sigma} = \partial \mathcal{E}<em>1 / \partial \rho</em>\sigma$</td>
<td>$\rho_{1\sigma} = -\partial \Omega_1 / \partial \rho_\sigma$</td>
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</table>

In perturbation theory, $T \to 0$ 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: $J = J_{hh} + J_{pp}$

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

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

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

- critical polarisation $P_c$: Thouless criterion

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

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 $\Sigma$:  
  \[ \text{→ jump } n_{p\to k_F^\sigma}^\sigma - n_{p\to k_F^\sigma}^\sigma = 1 + \frac{d}{d\omega} \Sigma^\sigma(\omega, k_F^\sigma) \bigg|_{\omega=\epsilon_F^\sigma} \]

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

  \( \text{(where } \epsilon_p^{\sigma*} = \epsilon_p^\sigma + \Sigma^\sigma(\epsilon_p^{\sigma*}, p) \))
Luttinger theorem

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

\[ \rightarrow \rho_{1\sigma} = \int \frac{d^3k}{(2\pi)^3} n_{1\sigma}^k = 0 \]

\[ \rightarrow \quad \begin{array}{ccc} \text{numbers of particles scattered out of their Fermi sea are equal for both spins} \\ \text{(weighted with } k^2) \end{array} \]

- satisfied in pp-RPA

- furthermore one can show: \[ \begin{array}{ccc} \text{numbers of particles scattered out of their Fermi sea are equal for both spins} \end{array} \]

- intuitively clear: ↑ and ↓ particles always scatter pairwise

- this explains why \( n_{k}^{\uparrow} \) is much more strongly modified than \( n_{k}^{\downarrow} \)
Chemical potentials and polaron energy

- NSR: $\mu$ is fixed, $\rho$ is changed $\iff$ here: $\rho$ is fixed, $\mu$ is changed

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

$\mu_\sigma$ vs. polarisation $P$:

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

Hartree: $\mu_\downarrow = (4\pi a/m)\rho_\uparrow$
there are extensions of the NSR scheme that avoid the problem in the polarised case by dressing propagators in $\Sigma$, 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 $\xi_{p\sigma}$

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

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

$$G_\sigma = G^*_\sigma + G^*_\sigma \Sigma_\sigma(\omega, p)$$

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

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

- additional approximation to simplify numerical implementation: constant shift $U_\sigma$ calculated at the Fermi surface

$$\xi^*_{p\sigma} \approx \epsilon_{p} - \mu_\sigma + U_\sigma, \quad U_\sigma = \text{Re} \Sigma_\sigma(\xi^*_{k_F\sigma}, k_F^\sigma), \quad \mu^*_\sigma = \mu_\sigma - U_\sigma$$
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 → missing screening correction (GMB)
- ZS: unrealistic dip in $T_c$ on the BEC side
- spin susceptibility at unitarity above $T_c$
  - $\chi_0$: 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 $\rho_1$ as a fct. of $T$

- within the ZS scheme, $\rho_1$ vanishes in the limit $T \rightarrow 0$
  \[ \rightarrow \text{ Luttinger theorem!} \]

- within NSR, effects from mean-field shift and correlations are mixed
  \[ \rightarrow \rho_{1\uparrow} \text{ and } \rho_{1\downarrow} \text{ stay finite for } T \rightarrow 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:
  \[ \exists k : \Gamma^{-1}(\omega = 0, k) = 0 \]

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

- problem: density correction

\[
\rho_1 = -\int \frac{d^3 k}{(2\pi)^3} \int \frac{d\omega}{\pi} g'(\omega) \left( \delta(\omega, k) - \frac{1}{2} \sin 2\delta(\omega, k) \right)
\]

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

\[ \Rightarrow \text{cannot describe transition at small } T \text{ and finite } P \]

- 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 $\rho_1$ 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
  $\rightarrow$ include correlated $n_p^\sigma$ into $\Gamma$ (“renormalised pp-RPA”)

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