Asymmetric Bethe-Salpeter equation - many phases of quantum gases

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Problems with paradigma of anomalous functions

Questions:

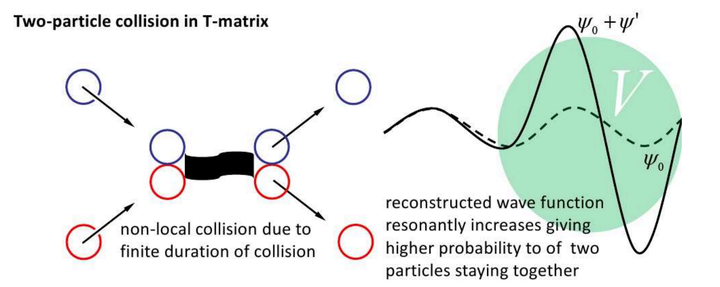
1. Why appears only one and not two condensates of cooper pairs?
2. Stability limited by pair excitation into bound pairs or pair breaking?
3. BEC and pairing transition treated on same theoretical basis?

Our view:

- Anomalous functions are short cut to right results (mean field), but same result possible without non-conserving assumptions
- Need unified theory above and below condensation temperature
- Fluctuations and condensation at same theoretical footing

Solution: T-matrix with multiple scattering corrections (MSC)

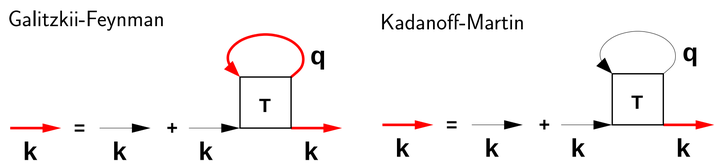
Many-body T-matrix



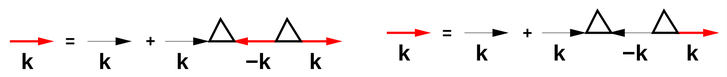
Scattered wave — reconstructed wave function — T-matrix

$$\Psi' = \frac{1}{E-H_0-V+i0}V\Psi_0 = \frac{V}{E-H_0+i0}V(\Psi_0+\Psi') = \frac{1}{E-H_0+i0}T\Psi_0$$

Dichotomy between gap and selfconsistency



Near pole (pairing, bound states) T-matrix is separable $T = \triangle\triangle$



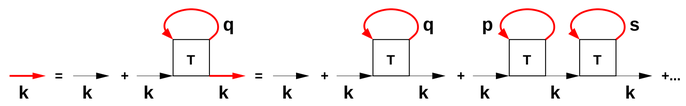
$G^{-1}(\omega,\mathbf{k}) = \omega + \epsilon_{\mathbf{k}} - \Delta^2 G(-\omega,-\mathbf{k})$ — no pole no gap equation

$G^{-1}(\omega,\mathbf{k}) = \omega + \epsilon_{\mathbf{k}} - \dfrac{\Delta^2}{\omega+\epsilon_{-\mathbf{k}}}$ — two-pole structure, BCS gap equation

- satisfying selfconsistency required by Goldstones criterion yield no gap
- theories giving gap do not satisfy selfconsistency

Removal of double counts

Paradox: The worse approximation yields better result
Wrong conclusion: Superconductor and metals not covered by unified theory
Solution: Galitskii-Feynman approximation includes double-counts



- Third particle ought to be different from the interacting pair: $p \neq q$!
- Each momentum contributes as 1/volume → vanishes for infinite volume
- Normal state ok, but pairing or BE condensates state $q \sim$ volume
- Derivation of asymmetric Bethe-Salpeter equation (cluster-cluster diagrams) K. Morawetz J. Stat. Phys. 143 (2011) 482

1. Phys. Rev. B 78 (2008) 214506: *Multiple scattering corrections to the T-matrix approximation: Unified theory of normal and superconducting states*, P. Lipavský
2. New J. Phys. 12 (2010) 033013: *Multiple condensed phases in attractively interacting Bose systems*, M. Männel, K. Morawetz, P. Lipavský
3. Phys. Rev. 82 (2010) 092501: *Equivalence of channel-corrected T-matrix and anomalous propagator approach*, K. Morawetz
4. J. Stat. Phys. 143 (2011) 482: *Asymmetric Bethe-Salpeter equation for pairing and condensation*, K. Morawetz
5. Phys. Rev. B 84 (2012) 094529: *Self-consistent T-matrix theory of superconductivity*, B. Šopík, P. Lipavský, M. Männel, K. Morawetz, P. Matlock
6. Phys. Rev. A 87 (2013) 053617: *Coexistence of phase transitions and hysteresis near the onset of Bose-Einstein condensation*, M. Männel, K. Morawetz, P. Lipavský,
7. Eur. Phys. J. B 87 (2014) 8: *Stability of condensate in superconductors*, P. Lipavský, K. Morawetz, B. Šopík, M. Männel

Subtraction of double counts

subtract own interaction in singular channel $G_{\backslash} = G - G_{\backslash}\Sigma_i G$
Using the Dyson equation $G_0^{-1} = G^{-1} + \Sigma$ $G_{\backslash} = G_0 + G_0(\Sigma - \Sigma_i)G_{\backslash}$

closing with the subtracted propagator $\Sigma_i = T_i\bar{G}_{\backslash}$, short exercise

$$G^{-1} = G_0^{-1} - \Sigma = G_0^{-1} - \Sigma' - \Sigma_i = G_0^{-1} - \Sigma' - T_i\bar{G}_{\backslash} = G_0^{-1} - \Sigma' - T_i\left(\bar{G}_0^{-1} - \bar{\Sigma}'\right)^{-1}$$

or explicitly

$$G = \frac{\bar{G}_0^{-1} - \bar{\Sigma}'}{[G_0^{-1} - \Sigma'][\bar{G}_0^{-1} - \bar{\Sigma}'] - T_i}$$

free propagator $G_0^{-1} = \omega - \epsilon_p$
"proper" selfenergy $\Sigma_{11}(p) \equiv \Sigma'(p)$
"anomalous" selfenergy $\Sigma_{12}(p) \equiv \Delta(p)$

in matrix form $\mathbf{G} = \mathbf{G^0} + \mathbf{G^0\Sigma G}$ with

$$\mathbf{G} = \begin{pmatrix} G_{11} & G_{12} \\ \bar{G}_{12} & \bar{G}_{11} \end{pmatrix},\ \mathbf{G_0} = \begin{pmatrix} G_0 & 0 \\ 0 & \bar{G}_0 \end{pmatrix},\ \mathbf{\Sigma} = \begin{pmatrix} \Sigma_{11} & \Sigma_{12} \\ \bar{\Sigma}_{12} & \pm\bar{\Sigma}_{11} \end{pmatrix}$$

Bosons S. T. Beliaev, Soviet. Phys. JETP 7 (1958) 289
Fermions L. P. Gorkov, Soviet. Phys. JETP 7 (1958) 505

"normal" $G_{11} \equiv G$ and "anomalous" Green' function

$$G_{12} \equiv \frac{-\Sigma_{12}}{(\omega+\epsilon+\bar{\Sigma}_{11})(\omega-\epsilon-\Sigma_{11})+\Sigma_{12}^2}$$

results, not needed as starting (conservation laws completed)
P. Lipavsky, PRB 78 (2008) 214506; K. Morawetz, PRB 82 (2010) 092501

Green function and particle density

- the dispersion has two branches $\pm E_q$

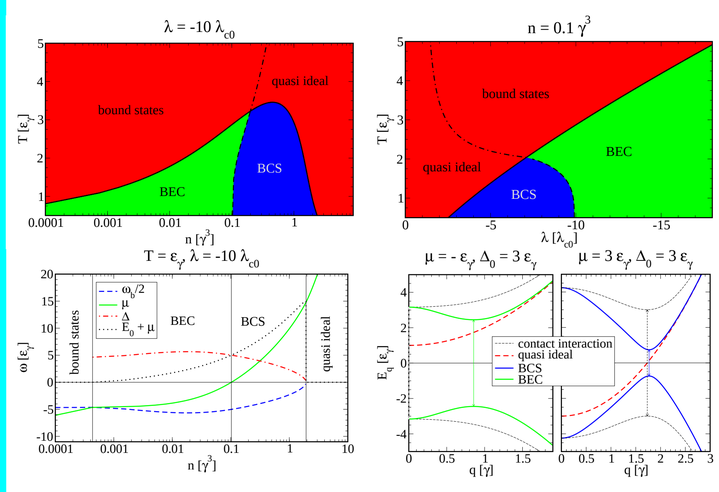
$$G(q,iz_\nu) = \frac{iz_\nu + \epsilon_q}{(iz_\nu)^2 - E_q^2},\quad E_q = \sqrt{\epsilon_q^2 \mp \Delta_0^2(q)},\quad \epsilon_q = \frac{\hbar^2 q^2}{2m} - \mu + \Sigma^{\rm reg}$$

- total density

$$n = \mp\frac{1}{\beta\Omega}\sum_{p,\nu} G(p,iz_\nu) = \pm\frac{1}{\Omega}\sum_p \frac{1}{2}\left[\frac{\epsilon_p}{E_p}\left(1 \pm 2f_{\rm B/F}(E_p)\right) - 1\right]$$

- solve many-body T-matrix for separable interaction $g_p = \left(1 + \frac{p^2}{\gamma^2}\right)^{-1}$
- pole of T-matrix yields binding energy $\omega_q < 0$ for pair,
- $\omega_0 = 2\mu$ (Thouless criterion), singular contribution condensation of Cooper pairs (BCS) but also condensation of bound states
- nonsingular contributions collected in regular self-energy $\Sigma^{\rm reg}$

Attractive Fermi gas



Stability of BCS condensate

excited bound states ($\mathbf{Q}$-mode), at zero frequency Cooper pairs ($\mathbf{C}$-mode), singular element $\mathcal{T}_{0,\mathbf{C}} = \frac{L^3}{k_{\rm B}T}\bar{\Delta}\Delta$, T-matrix of the condensation mode $\mathcal{T}_{0,\mathbf{C}} = V - V\frac{k_{\rm B}T}{L^3}\sum_k G_\uparrow(\omega,\mathbf{k})G_\downarrow(-\omega,\mathbf{C}-\mathbf{k})\mathcal{T}_{0,\mathbf{C}}$

near T_c T-matrix diverges, expand (GL equation Gorkov)

$$\frac{\hbar^2|\mathbf{C}|^2}{2m^*}\bar{\Delta} + \alpha\bar{\Delta} + \beta|\Delta|^2\bar{\Delta} = 0$$

T-matrix $\frac{1}{\mathcal{T}_{0,\mathbf{Q}}} = \frac{1}{V} + \frac{k_{\rm B}T}{L^3}\sum_k G_\uparrow(\omega,\mathbf{k})G_\downarrow(-\omega,\mathbf{Q}-\mathbf{k})$ for non-condensed pairs both propagators depend on gap, leads to energy

$$\frac{\chi}{\mathcal{T}_{0,\mathbf{Q}}} = \frac{|\mathbf{Q}|^2}{2m^*} + \alpha + 2\beta|\Delta|^2$$

in condensation mode $\frac{\chi}{\mathcal{T}_{0,\mathbf{C}}} = \frac{|\mathbf{C}|^2}{2m^*} + \alpha + \beta|\Delta|^2 = 0$ identical to GL approximation, eliminate gap $\frac{\chi}{\mathcal{T}_{0,\mathbf{Q}}} = \frac{|\mathbf{Q}|^2}{2m^*} - \alpha - \frac{|\mathbf{C}|^2}{m^*}$, zero only if $|\mathbf{C}|^2$ compensate $-\alpha$

- T-matrix in the $\mathbf{Q}$-mode remains finite, cannot become singular once the condensation develops in $\mathbf{C}$-mode
- factor of two in non-linear term: non-condensed pairs feel gap due to condensate twice stronger than by Cooper pairs in condensate (like bosons out of BEC twice stronger)
- therefore parallel condensation in two competitive modes is excluded (tacitly assumed in BCS theory)

Excitation of Cooper pairs from the condensate

N particles (Cooper pairs) in running frame $\mathbf{v}$ excite quasiparticle (bound pair) ϵ_Q, possible if (Cherenkov) $E_i - E_f = \mathbf{v}\cdot\mathbf{Q} - (\epsilon_Q - \epsilon_0) > 0$, i.e.

$(\mathbf{v}\cdot\mathbf{Q}) \geq \frac{\chi}{\mathcal{T}_{0,\mathbf{Q}}} = \frac{|\mathbf{Q}|^2}{2m^*} - \alpha - \frac{|\mathbf{C}|^2}{m^*}\Big|_{C=0} = \frac{|\mathbf{Q}|^2}{2m^*} - \alpha$ solved by real $\mathbf{Q}$ only if $|\mathbf{v}| > v_{\rm pe} = \sqrt{\frac{2|\alpha|}{m^*}}$ since pair breaking velocity $v_{\rm pb} = \frac{\Delta}{k_{\rm F}} = \sqrt{\frac{|\alpha|}{\beta k_{\rm F}}} = \sqrt{\frac{|\alpha|}{3m}}$ we have the relation

$$v_{\rm pe} = \sqrt{3}v_{\rm pb}$$

- critical velocity of pair breaking < critical velocity of pair excitation → stability of condensate controlled by pair breaking
- The Galitskii-Feynman T-matrix approximation fails for superconducting state because of non-physical repeated collisions
- MSC -Tmatrix theory of pairing and condensation is valid above and below critical temperature: consistent description of pair-breaking effects
- MSC T-matrix justifies two basic assumptions of BCS theory: condensate single-valued, excitations of bound electron pairs can be neglected

	critical velocities of pair breaking	critical velocities of pair excitation
Galitskii	0	0
KM	$\Delta/k_{\rm F}$	0
TMSC	$\Delta/k_{\rm F}$	$\sqrt{3}\Delta/k_{\rm F}$

Approximations for Bose gases

The total energy in T-matrix approximation is

$$U = \underbrace{\sum_{k\neq 0} E_k f_{\rm B}(E_k)}_{\text{quasi particles}} + \underbrace{\sum_{k\neq 0}\frac{n_0^2\mathcal{T}^2(k)}{4E_k}(1+2f_{\rm B}(E_k))}_{\text{two-particle contribution}} - \underbrace{\sum_{k\neq 0} E_k v_k^2}_{\text{depletion}} + \underbrace{\frac{\mathcal{T}(0)}{\Omega}\left(N^2 - NN_0 + \tfrac{1}{2}N_0^2\right)}_{\text{attraction in momentum space}}$$

and the total number of particles is

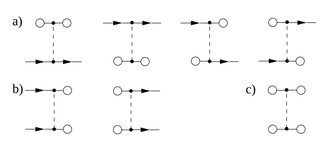
$$N = N_0 + \underbrace{\sum_{k\neq 0} f_{\rm B}(E_k)}_{\text{quasi particles}} + \underbrace{\sum_{k\neq 0} v_k^2(1+2f_{\rm B}(E_k))}_{\text{depletion}}$$

I. Hartree-Fock
$n = n^{\rm id},\quad \mu = \mu^{\rm id} + 2nU_0$ for $n_0 = 0$
$n = n_0 + \Delta n,\ \mu = (2n - n_0)U_0$ for $n_0 > 0$

II. Bogoliubov
attraction in momentum space, correlations, $\mu \approx n_0 U_0$

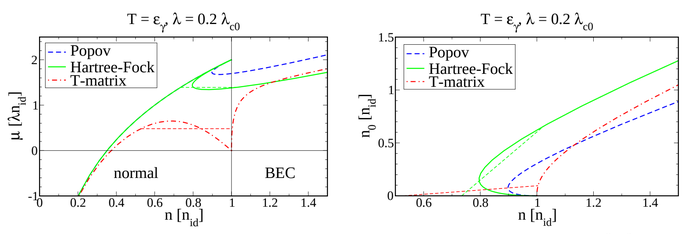
$$E = \sum_k E_k f_{\rm B}(E_k) + \frac{N_0U_0}{2\Omega}(2N - N_0) - \sum_{k\neq 0} E_k v_k^2$$

$$E_k = \sqrt{\left(\frac{\hbar^2k^2}{2m} + n_0U_0\right)^2 - n_0^2U_0^2}$$



III. Popov (Hartree-Fock-Bogoliubov): $\mu = (2n - n_0)U_0$

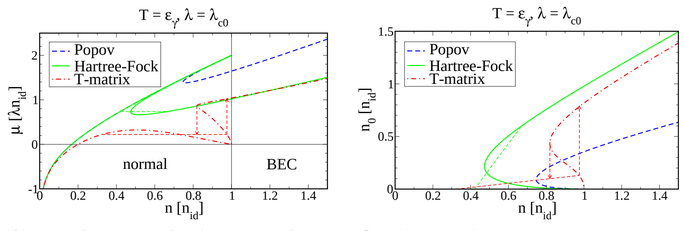
Weak repulsive-interacting Bose gas



Chemical potential with ideal critical density $n_{id} \approx 0.059\gamma^3$ — Condensate density, $\varepsilon_\gamma = \hbar^2\gamma^2/2m$, $\lambda_{c0} = 8\pi\hbar^2/m\gamma$

- Popov and Hartree-Fock approximation show unphysical behavior due to overestimation of attraction in momentum space
- instability at onset of BEC and first-order phase-transition (Maxwell construction)
- T-matrix approximation medium effects compensate repulsive interaction near onset of BEC, attraction in momentum space compensated, nevertheless first-order phase-transition
- in coexistence region condensate density changes linearly

Strong repulsive-interacting Bose gas



Chemical potential, the vertical arrows mark the density hysteresis — Condensate density

- for strong repulsive interaction the attraction in momentum space is too strong to be compensated by medium effects
- also T-matrix approximation yields multivalued region, which cannot be avoided by the Maxwell construction
- therefore a true physical relevance is attributed to this behavior and it is interpreted as appearance of a hysteresis