Weighted Hartree-Fock-Bogoliubov method for interacting fermions

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To the paper

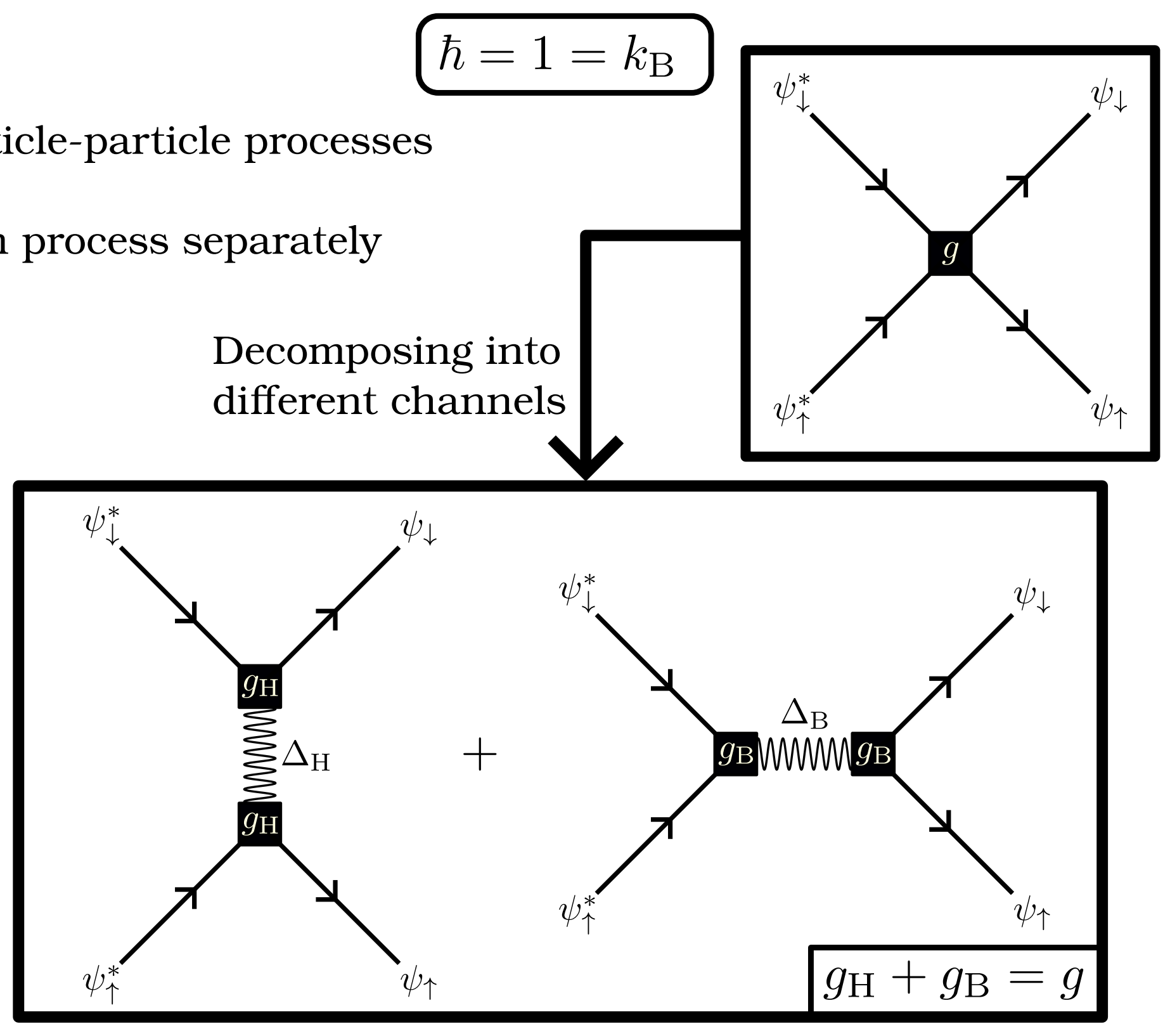
Partitioning of interaction channels

- Hamiltonian density: $\mathcal{H} - \mu\mathcal{N} = \sum_{\sigma\in\mathcal{S}} \psi^*_\sigma(x)\Big[-\frac{\nabla^2}{2m} - \mu\Big]\psi_\sigma(x) - g\psi^*_\uparrow(x)\psi^*_\downarrow(x)\psi_\downarrow(x)\psi_\uparrow(x)$

$\boxed{\hbar = 1 = k_\mathrm{B}}$

- Interaction separates in particle-hole and particle-particle processes
- Hubbard-Stratonovich transformation for each process separately
- Distinct coupling constants g_H and g_B
- Two auxiliary fields to describe interactions

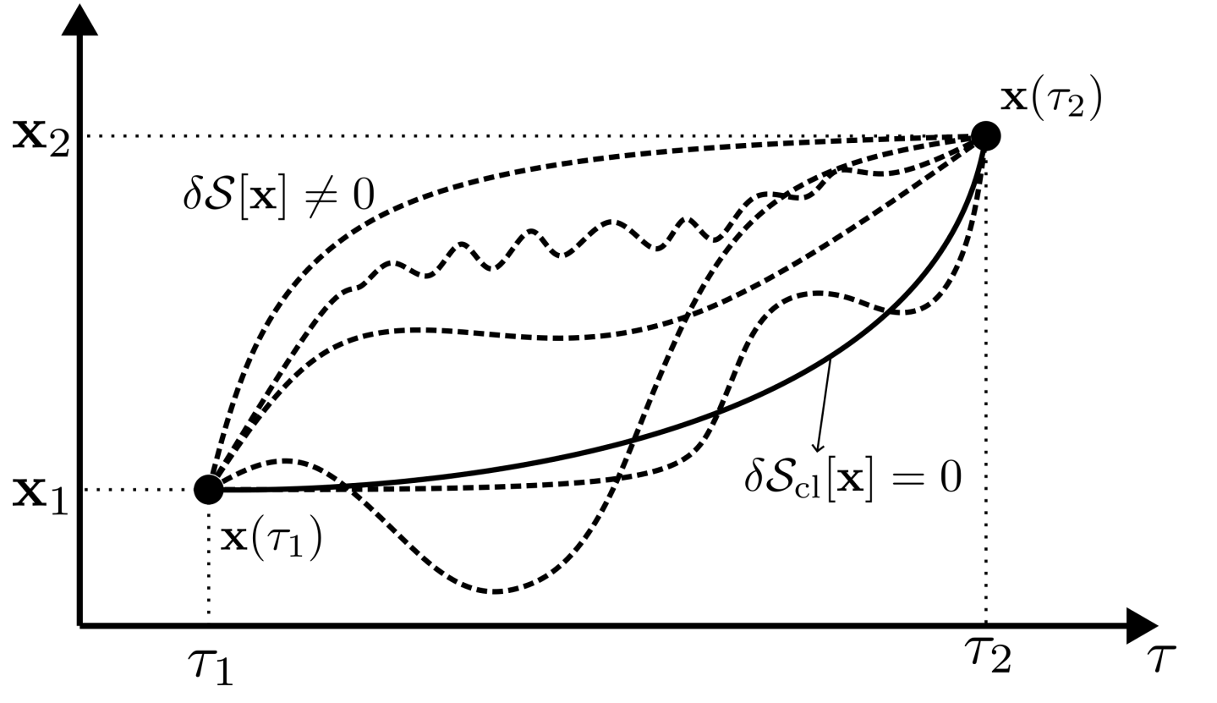
Δ_H	Δ_B
Real field	Complex field
Connected to density	Connected to pairs
$\propto \langle\psi^*_\uparrow\psi_\uparrow + \psi^*_\downarrow\psi_\downarrow\rangle$	$\propto \langle\psi_\downarrow\psi_\uparrow\rangle$
Particle-hole process	Particle-particle process
=> Normalfluid	=> Superfluid


Decomposing into different channels

$g_\mathrm{H} + g_\mathrm{B} = g$

Application of WHFB theory to cold attractive Fermi systems

Classical example:



- Action functional of path, minimization yields classical physics
- Fluctuations around classical path contribute less

=> Feynman path integration

Generalization to fields
=> Space and time as parameters

Field minimization:

- Decompose into classical path and quantum fluctuations

$$\Delta_\mathrm{H}(\tau;\mathbf{x}) = \boxed{\Delta_{\mathrm{H},0}} + \boxed{\eta_\mathrm{H}(\tau;\mathbf{x})}$$
$$\Delta_\mathrm{B}(\tau;\mathbf{x}) = \boxed{\Delta_{\mathrm{B},0}} + \boxed{\eta_\mathrm{B}(\tau;\mathbf{x})}$$

Quantum fluctuations
Space-time dependence

=> $\mathcal{S}_\mathrm{eff}[\Delta_\mathrm{H};\Delta_\mathrm{B}] = \mathcal{S}_\mathrm{MF}[\Delta_{\mathrm{H},0};\Delta_{\mathrm{B},0}] + \mathcal{S}_\mathrm{fluct}[\Delta_{\mathrm{H},0};\Delta_{\mathrm{B},0};\eta_\mathrm{H};\eta_\mathrm{B}]$

Saddle Point => Mean-Field solution
Static and uniform

- Minimize grand-canonical potential $\Omega_\mathrm{MF} = -T\log\mathcal{Z}_\mathrm{MF} = T\mathcal{S}_\mathrm{MF}[\Delta_{\mathrm{H},0};\Delta_{\mathrm{B},0}]$

$$\Delta_{\mathrm{H},0} = -\frac{g_\mathrm{H}}{2}n$$

$$\Delta_{\mathrm{B},0} = g_\mathrm{B}\Delta_{\mathrm{B},0}\frac{1}{V}\sum_\mathbf{k}\frac{\tanh\left(\frac{E_\mathbf{k}}{2T}\right)}{2E_\mathbf{k}}$$

Bogoliubov dispersion

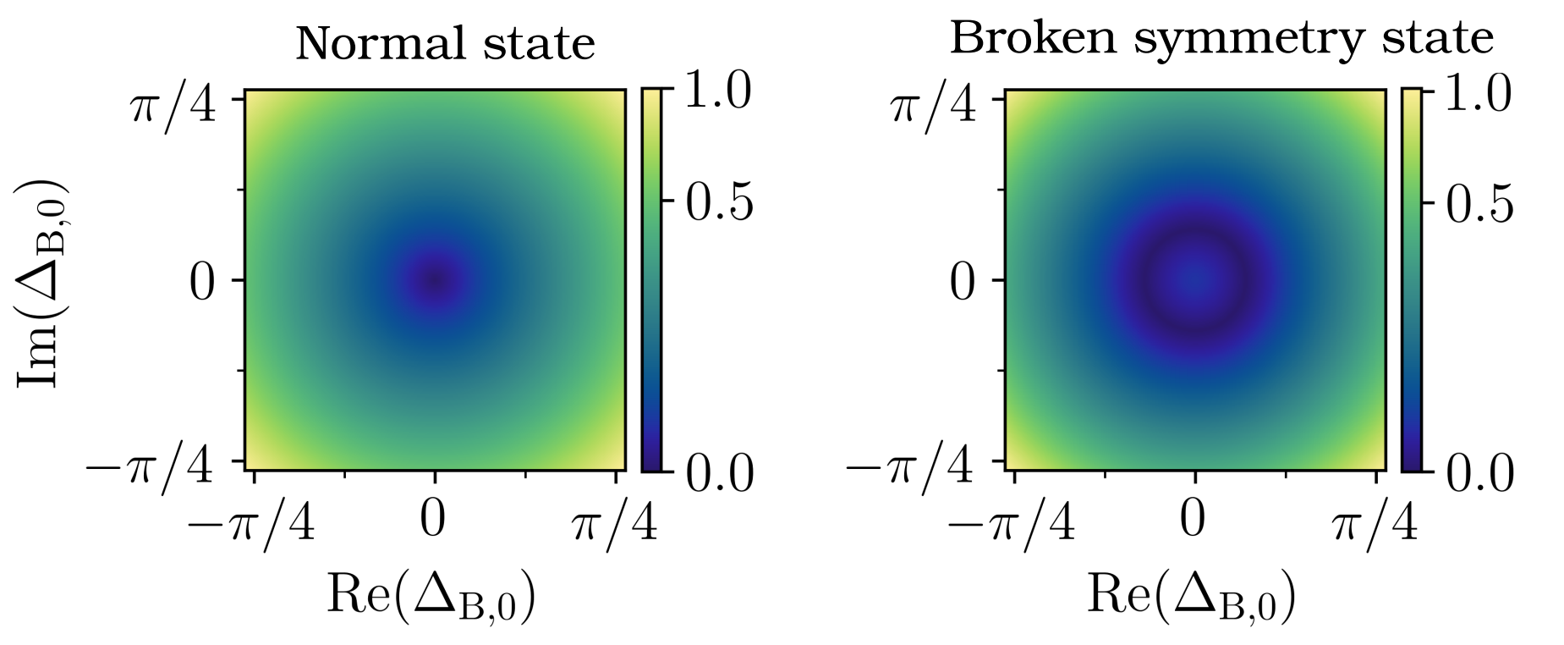
$$E_\mathbf{k} = \sqrt{\left(\frac{k^2}{2m} - \mu + \Delta_{\mathrm{H},0}\right)^2 + |\Delta_{\mathrm{B},0}|^2}$$

Extremization of thermodynamic potential w.r.t. weighted interaction strengths yields

$$g_\mathrm{H} = \frac{|\Delta_{\mathrm{H},0}|}{|\Delta_{\mathrm{H},0}| + |\Delta_{\mathrm{B},0}|}g = h_0 g$$

$$g_\mathrm{B} = \frac{|\Delta_{\mathrm{B},0}|}{|\Delta_{\mathrm{H},0}| + |\Delta_{\mathrm{B},0}|}g = b_0 g$$

Two types of potentials for superfluid order parameter [4]



Trivial solution ($T > T_\mathrm{C}$) Superfluid solution ($T < T_\mathrm{C}$)

Particle-hole order parameter has no broken symmetry
Minimization of energy however yields kink in free energy

Renormalization Scheme

- Lippmann-Schwinger equation for microscopic spherical symmetric scattering processes [5,6]

$$q\cot\delta_0(\mathbf{q}) = -\frac{1}{a_\mathrm{s}} + \frac{1}{2}r_\mathrm{e}q^2 + \mathcal{O}(q^4)$$

Scattering momentum
s-wave scattering phase shift
Effective range parameter
s-wave scattering length

- Contact potential scattering phase shift:

$$q\cot\delta_0(\mathbf{q}) = \boxed{\frac{4\pi}{mg} - \frac{2\Lambda}{\pi}} + \boxed{\frac{2}{\pi\Lambda}q^2} + \mathcal{O}(q^4)$$

Characteristic unit system:
Fermi units
$\varepsilon_\mathrm{F} = T_\mathrm{F} = k_\mathrm{F}^2/2m$

Leading order coefficients:

$$\frac{1}{g(\Lambda)} = -\frac{m}{4\pi a_\mathrm{s}} + \frac{m}{2\pi^2}\Lambda$$
$$= -\frac{m}{4\pi a_\mathrm{s}} + \sum_\mathbf{k}^\Lambda \frac{m}{\mathbf{k}^2}$$

Divergence for infinite cut-off cancels scattering divergence in pairing field equation

Next Leading Order (NLO)
Identification of UV cut-off:

$$\Lambda(r_\mathrm{e}) = \frac{4}{\pi r_\mathrm{e}}$$

Physical significance of UV cut-off

- Allows inclusion of NLO range effects
- Keeps pairing equation finite
- Range to zero recovers standard theory
- Example ^{6}Li: $r_{\mathrm{e,s}} \approx 87\,a_0$ [5]

$\mathcal{O}(q^0)$
Regularization of divergence

Superfluid order parameter

$$\frac{m}{4\pi a_\mathrm{s}} = \sum_\mathbf{k}^{\Lambda(r_\mathrm{e})}\left[\frac{m}{\mathbf{k}^2} - \frac{\tanh\left(\frac{\beta}{2}E_\mathbf{k}\right)}{2E_\mathbf{k}}\right]$$

Hartree order parameter

$$\Delta_\mathrm{H} = \min\left(\frac{4\varepsilon_\mathrm{F}/3\pi}{\frac{1}{k_\mathrm{F}a_\mathrm{s}} - \frac{8}{\pi^2 k_\mathrm{F} r_\mathrm{e}}} + |\Delta_\mathrm{B}|; 0\right)$$

$\mathcal{O}(q^2)$
Inclusion of effective range

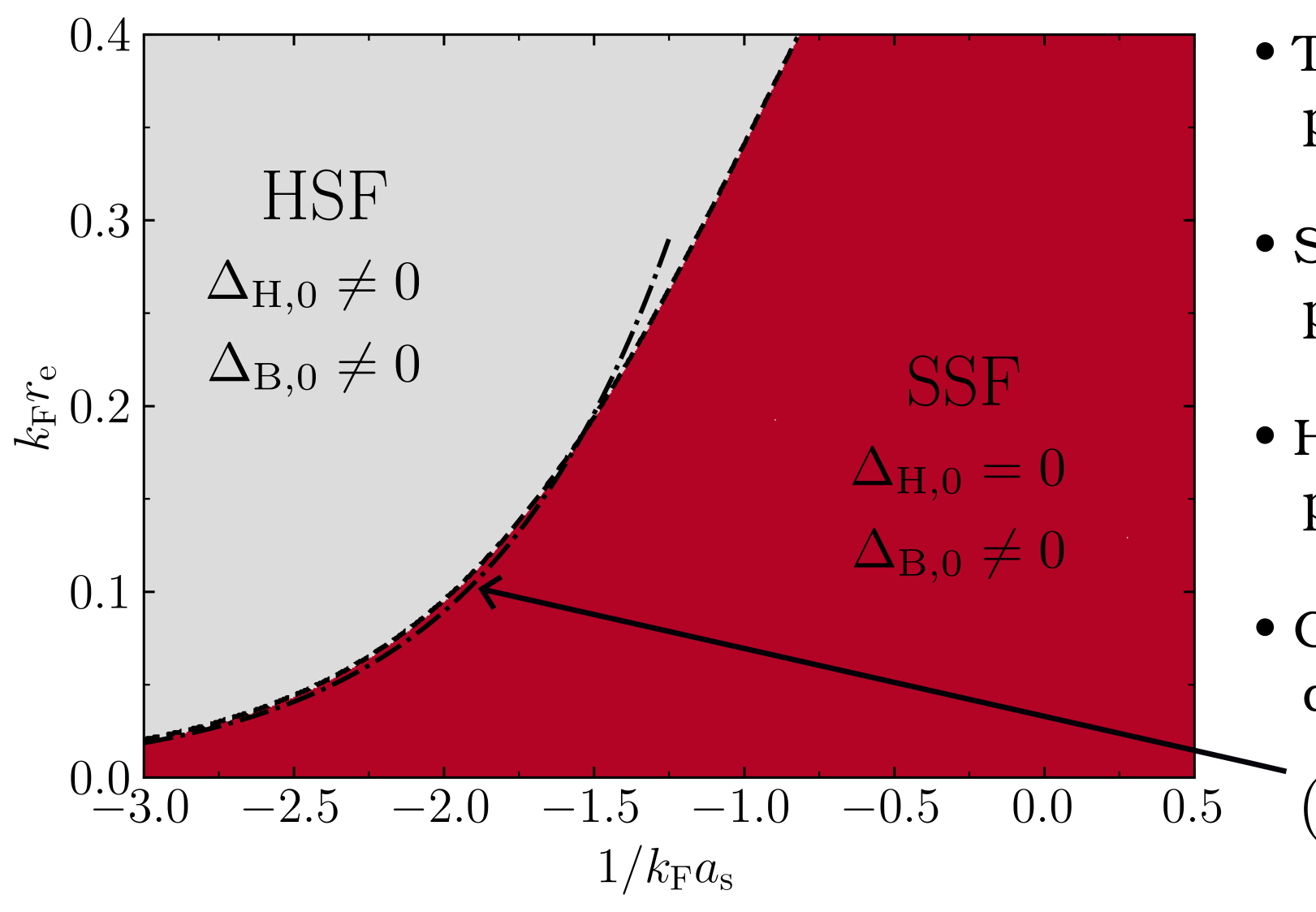
Abstract

For several decades it has been known that divergences arise in the ground-state energy and chemical potential of unitary superfluids, where the scattering length diverges, due to particle-hole scattering. Leading textbooks [1] and research articles [2,3] recognize that there are serious issues but ignore them due to the lack of an approach that can regularize these divergences. We find a solution to this difficulty by proposing a general method, called the weighted Hartree-Fock-Bogoliubov (WHFB) theory, to handle multiple decomposition channels originating from the same interaction. We distribute the interaction in weighted channels determined by minimization of the action, and we apply this idea to unpolarized Fermi superfluids. Using our method, we solve a long-standing difficulty in the partitioning of the interaction into Hartree, Fock, and Bogoliubov channels for Fermi superfluids.

We emphasize that our method is so general, that it can be applied to any fermionic system that can support competing interaction channels. This includes systems from particle and nuclear physics, condensed matter physics, ultracold atoms, and even astrophysical objects like the crusts of neutron stars.

Ground State ($T = 0$)

Ground State Phase Diagram



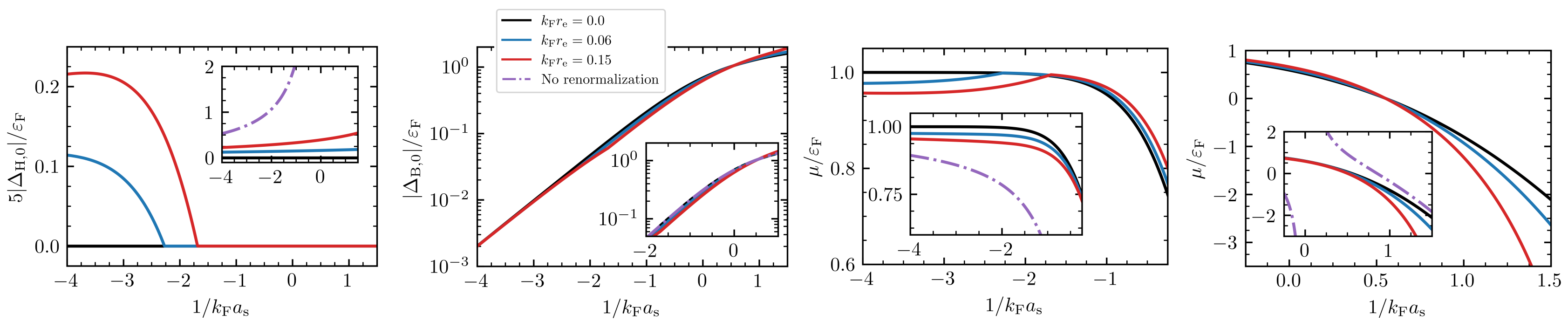
- Two phases even in ground state, depending on range parameter
- SSF as standard superfluid without particle-hole process
- HSF as Hartree-superfluid having both order parameters assume finite values
- Critical range parameter corresponds to a critical density below which pairing is preferred

$$(k_\mathrm{F}r_\mathrm{e})_\mathrm{crit} \sim \exp\left(-\frac{\pi}{2|k_\mathrm{F}a_\mathrm{s}|}\right)$$

Order parameters

- Particle-hole order parameter goes to zero for strong interactions
- Reduction of superfluid order parameter due to interaction range

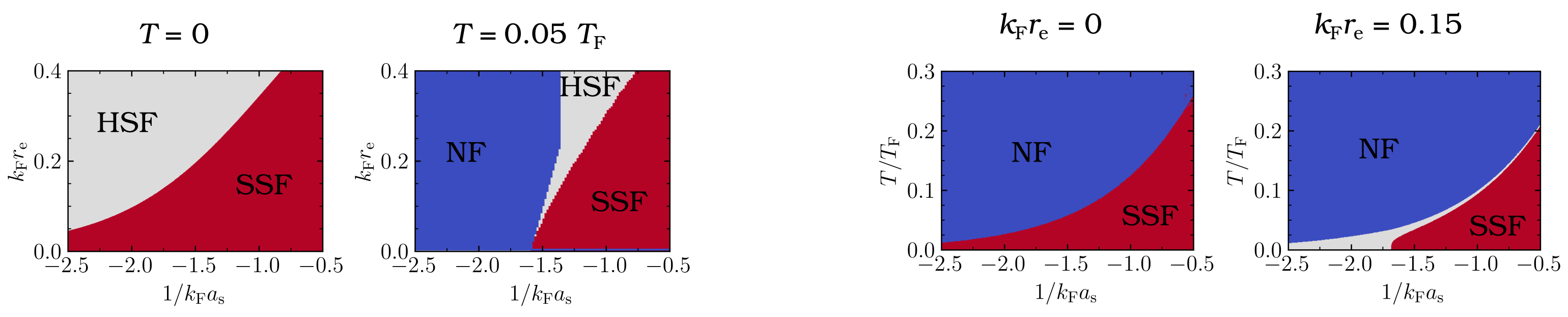
Effects increase with increasing effective range parameter
=> Also higher densities



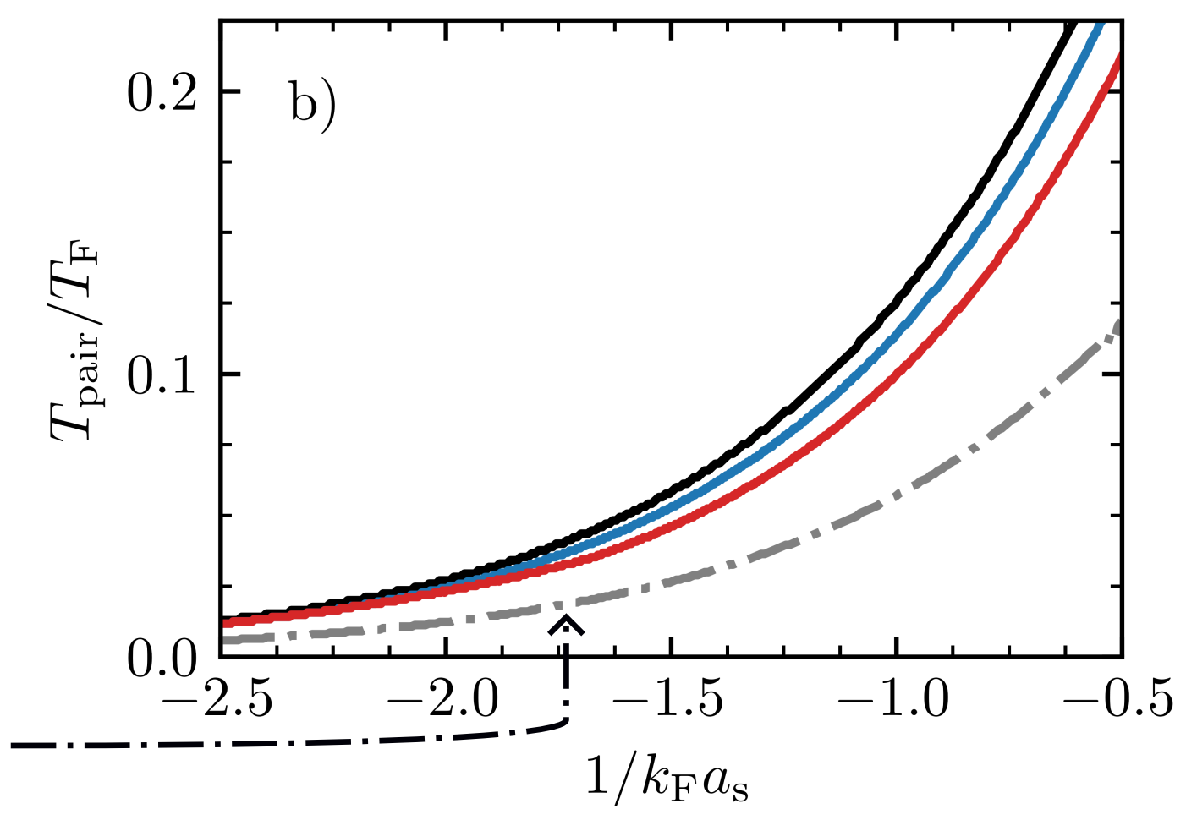
- Chemical potential gets reduced by particle-hole channel up to critical interaction strength
- Weakly interacting gas dominated by particle-hole processes, instead of pairing processes from Refs. [4,8]
- Stronger interaction favors pair-processes by particle-particle processes

Finite-Temperature Effects

Fixed temperature Fixed effective range



- At finite temperatures normal fluid (NF) regime dominated particle-hole processes emerges
- SSF and NF phases are each dominated by one order parameter, intermediate HSF has both
- At higher T there exist scattering lengths that are always capable of having particle-hole interaction
- Reduction of superfluid T_pair for increasing effective range, close to Gor'Kov and Melik-Bhakudarov theory [7]



Conclusion

- Self-consistent treatment of multiple interaction channels possible by WHFB method
  => Successful inclusion of particle-hole channels into theoretical description
- Minimization of free energy with respect to weights yields non-perturbative coupling between particle-hole (Hartree) and superfluid (Bogoliubov) order parameter
- Weakly-interacting gas is dominated by particle-hole processes -> Reduction of superfluid order parameter
- Reduction of pair temperature -> Step towards GMB fluctuation corrections [9] even at mean-field

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