Pair coherence and healing lengths for a fermionic superfluid throughout the BCS-BEC crossover

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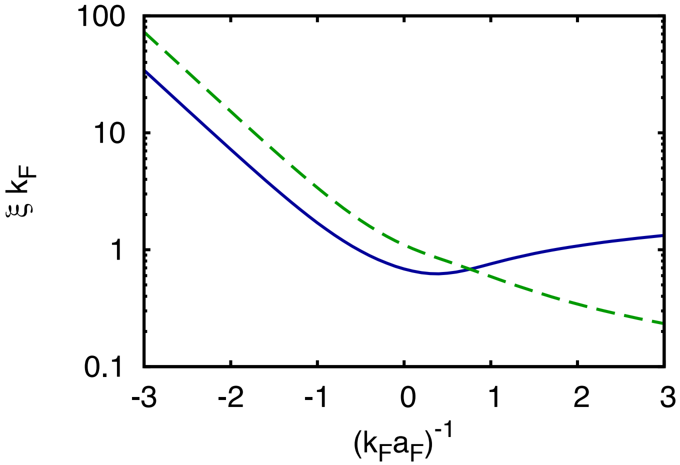
Subtitle: “Les trois longueurs de la supra-conductivité - Vingt ans aprè”

⋆ Work done with F. Palestini [PRB **89**, 224508 (2014)]

- The lengths relevant to superconductivity are:
  - the intra-pair coherence length $\xi_{\rm pair}$
  - the inter-pair coherence length $\xi_{\rm phase}$
  - the inter-particle distance k_F^{-1}
- $\xi_{\rm pair}$ at $T = 0$ was calculated throughout the BCS-BEC crossover by F. Pistolesi and GCS [PRB **49**, 6356 (1994)]
- Soon after, also $\xi_{\rm phase}$ at $T = 0$ was calculated throughout the BCS-BEC crossover by FP-GCS [PRB **53**, 15168 (1996)]

ξ_{pair} and ξ_{phase} at $T = 0$ vs the coupling:

Here are the results that go twenty years back:



ξ_{pair} = - - - - - ξ_{phase} = ———

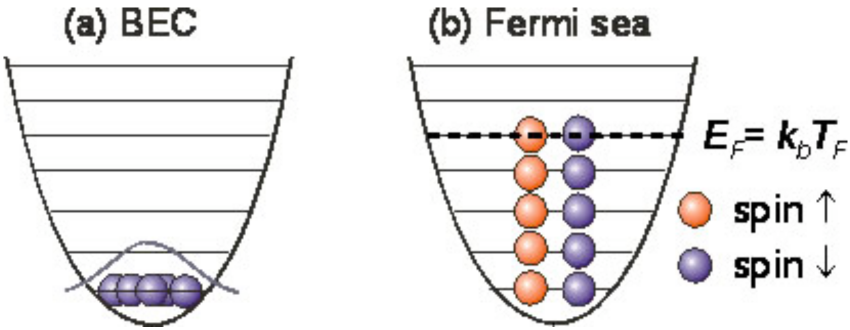
“Twenty years later” we have extended the results at finite T (also above T_c):

ξ_{pair} $\quad$ k_F^{-1} $\quad$ ξ_{phase}

Realization of the BCS-BEC crossover:

$(k_F a_F)^{-1} \gtrsim +1$ $\qquad$ $(k_F a_F)^{-1} \lesssim -1$

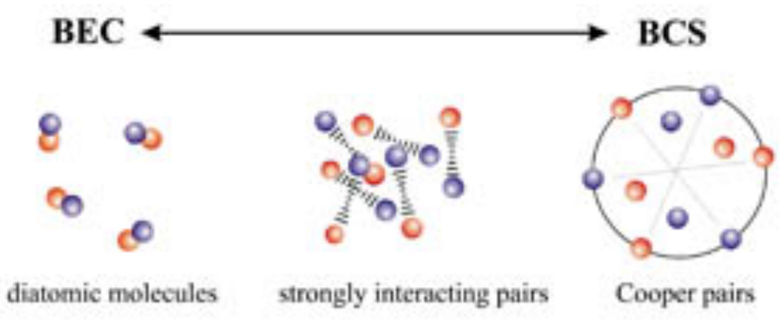
$(k_F$ = Fermi wave vector$)$



… that is, dimers vs Cooper pairs:

$+1.0$ $\qquad$ 0.0 $\qquad$ -1.0

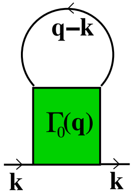
$(\mathbf{k_F\, a_F})^{-1}$

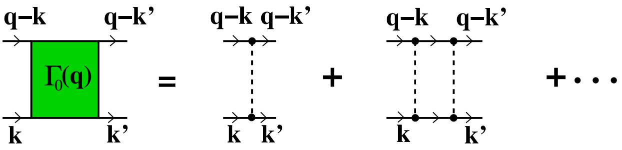


unitarity point $(\mathbf{k_F\, a_F})^{-1} = 0 \quad \Longleftrightarrow \quad$ universality !

Extension to finite T $\rightarrow$ the t-matrix:

Pairing fluctuations beyond mean field are required at finite T (definitely above T_c) $\Rightarrow$ the t-matrix Γ_0





How is $\xi_{\rm pair}$ defined ?

- $\xi_{\rm pair}$ is obtained from the *pair correlation function* for opposite-spin fermions:

$$
\begin{aligned}
g_{\uparrow\downarrow}(\boldsymbol{\rho}) \;=\; & \left\langle \psi^\dagger_\uparrow\left(\mathbf{R}+\frac{\boldsymbol{\rho}}{2}\right)\psi^\dagger_\downarrow\left(\mathbf{R}-\frac{\boldsymbol{\rho}}{2}\right)\psi_\downarrow\left(\mathbf{R}-\frac{\boldsymbol{\rho}}{2}\right)\psi_\uparrow\left(\mathbf{R}+\frac{\boldsymbol{\rho}}{2}\right)\right\rangle \\
& - \;\left(\frac{n}{2}\right)^2
\end{aligned}
$$

$\boldsymbol{\rho} = \mathbf{r} - \mathbf{r}'$ relative coordinate

$\mathbf{R} = (\mathbf{r} + \mathbf{r}')/2$ center-of-mass coordinate, such that

$$\xi^2_{\rm pair} = \frac{\int d\boldsymbol{\rho}\, \boldsymbol{\rho}^2\, g_{\uparrow\downarrow}(\boldsymbol{\rho})}{\int d\boldsymbol{\rho}\, g_{\uparrow\downarrow}(\boldsymbol{\rho})} \, .$$

How is ξ_{phase} defined ?

- ξ_{phase} is obtained from the (static) *correlation function of the order parameter* :

$$F_{\parallel}(\mathbf{R}-\mathbf{R}') = \int_0^{\beta} d\tau \, \langle T_{\tau} \left[\varphi_{\parallel}(\mathbf{R},\tau)\varphi_{\parallel}(\mathbf{R}',\tau=0) \right] \rangle - \beta \, |\Delta|^2$$

$\beta = (k_B \, T)^{-1}$ and $\varphi_{\parallel}(\mathbf{R}) = \frac{1}{2|\Delta|} \left[\Delta^* \varphi(\mathbf{R}) + \Delta \varphi^{\dagger}(\mathbf{R}) \right]$

where $\varphi(\mathbf{R}) = v_0 \psi_{\downarrow}(\mathbf{R}) \psi_{\uparrow}(\mathbf{R})$ such that $\langle \varphi(\mathbf{R}) \rangle = \Delta$

(v_0 = strength of the attractive inter-particle interaction).

Obtaining these two correlations functions for $\xi_{\rm pair}$ and $\xi_{\rm phase}$ in terms of a diagrammatic structure :

Above T_c, the two correlation functions can be obtained in terms of the same diagrammatic structure :

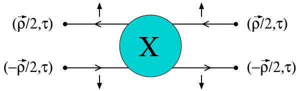
(a) $\longleftrightarrow$ $\xi_{\rm pair}$

(b) $\longleftrightarrow$ $\xi_{\rm phase}$

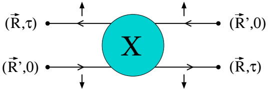
$\Longleftarrow$ the minimal ingredient is the series of "maximally crossed diagrams" X **(c)**.

Note that only the external variables are different in the two cases !

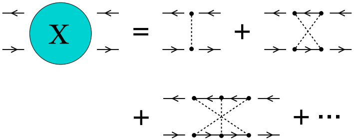
(a)



(b)



(c)



Main results (mostly above T_c) :

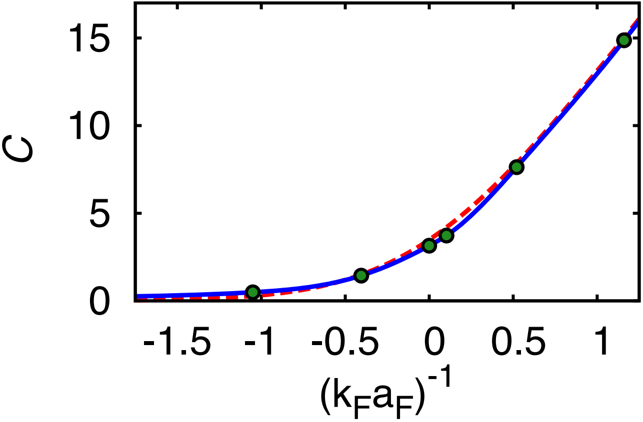
- At short distances, $g_{\uparrow\downarrow}(\boldsymbol{\rho})$ is given by:

$$g_{\uparrow\downarrow}(\boldsymbol{\rho}) \xrightarrow[(\boldsymbol{\rho}\to 0)]{} \left(\frac{m}{4\pi}\right)^2 \int dq\, e^{i\Omega_\nu \eta}\, \Gamma_0(q) \left(\frac{1}{\rho^2} - \frac{2}{a_F \rho}\right)$$

where $m^2 \int dq\, e^{i\Omega_\nu \eta}\, \Gamma_0(q)$ is identified with

the Tan's contact C $\Longrightarrow$ universality !

That is to say, the same result for C should be obtained, e.g., also from the tail of the wave-vector distribution $n(\mathbf{k})$ (here, results at $T = 0$):



- - - - BCS mean field - $C_{BCS} = (m\,\Delta_{BCS})^2$

—— plus pairing fluctuations

• from the tail of $n(\mathbf{k})$

And what about the “nuclear” contact?

The Nuclear Contact Exists

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(Dated: July 31, 2014)

Many-body systems of strongly interacting Fermions are ubiquitous in nature, ranging from High-Tc superconductors and ultra-cold atomic gases to atomic nuclei and neutron stars. Theoretical predictions, recently verified by measurements on ultra-cold atomic gases, show that under certain conditions the universal behavior of systems composed of two kinds of fermions can be described using a single parameter, simply called the contact, which is a measure of the number of different-fermion pairs in close proximity. This paper discusses the relevance of the contact for very different systems: atomic nuclei, made of strongly-interacting neutrons and protons. Here we show that the high-momentum distributions of protons and neutrons in nuclei, dominated by correlated proton-neutron pairs mainly in a spin-triplet state, have the same momentum dependence as those of cold atoms, with a strength described by the contact. We use high-energy electron scattering data to extract a value for the nuclear contact consistent with that observed for atomic gases. This means that, when the scaled interaction strength of the atomic system is chosen to be equal to that in nuclei, the probabilities of finding a correlated high-momentum different-fermion pair in both systems is about 20%. Atomic nuclei are self-bound, strongly-interacting systems with a density that is about 25 orders of magnitude larger than of trapped cold atomic gases, so the ability to describe the correlations in both systems by the same parameter is remarkable and unexpected.

(from arXiv:1407.8175v1 [nucl-ex] 30 July 2014)

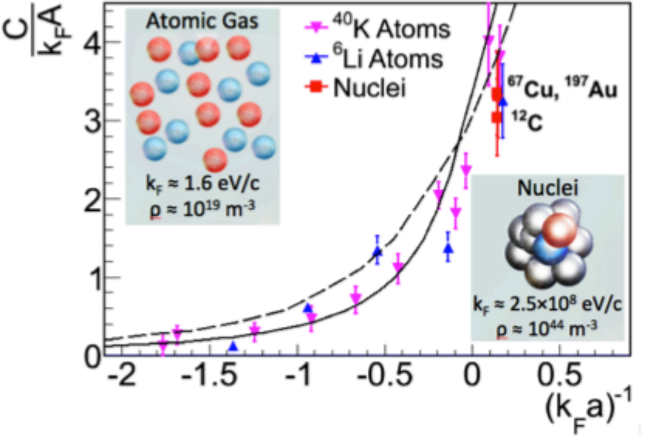


FIG. 3: The contact plotted versus $(k_F a)^{-1}$, the inverse of the product of the scattering length and Fermi momentum, as extracted from measurements of ultra-cold two-spin state atomic systems [5, 6] and atomic nuclei (see Table I). The dashed and solid lines are the theoretical predictions of Refs. [32] and [33] respectively.

- Through its spatial oscillations, $g_{\uparrow\downarrow}(\rho)$ provides also information about the underlying Fermi surface (if any).

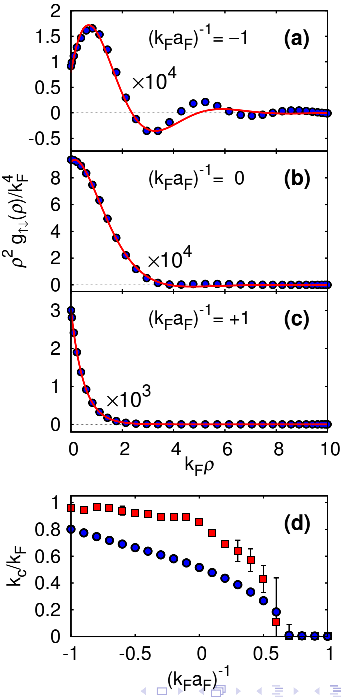
The numerical results for $\rho^2\, g_{\uparrow\downarrow}(\rho)$ at T_c are fitted by:

$$f(\rho) \;=\; A\cos(\phi_0 + \sqrt{2}\rho k_c) \times e^{-\sqrt{2}\rho/\ell_0}$$

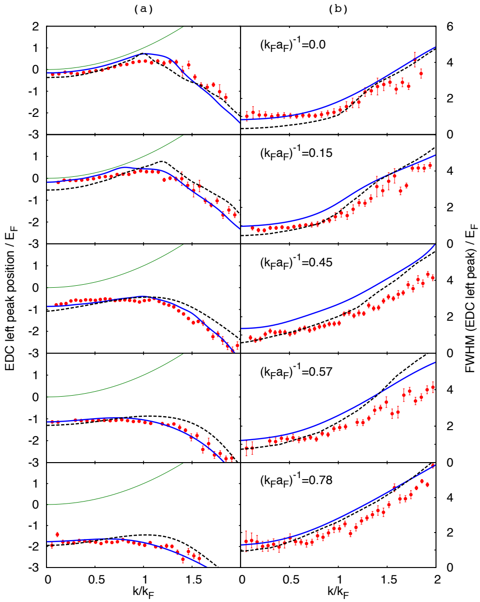
for different couplings $\Longrightarrow$

Obtain k_c vs $(k_F\, a_F)^{-1}$ ●

Compare it with a similar wave vector k_L obtained from momentum-resolved radio-frequency spectra ■



N.B. In PRL **106**, 060402 (2011) the (*Luttinger*) *wave vector* k_L was extracted from the experimental (with fermionic ^{40}K ultra-cold atoms) and theoretical energy distribution curves (EDCs) obtained at T_c for several couplings. The wave vector k_L marks the place where the "backbending" occurs in the EDCs. When this backbending disappears, k_L vanishes.



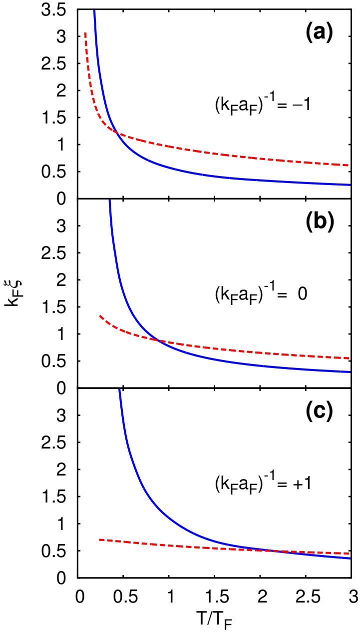
- At any coupling, $\xi_{\rm pair}$ has a finite value at T_c and is a decreasing function of temperature.

- At high temperatures, $\xi_{\rm pair} \simeq \frac{1}{\sqrt{2\, m\, k_B\, T}} = \frac{\lambda_T}{\sqrt{4\,\pi}}$ where λ_T is the *thermal wavelength*.

- Close to T_c, $\xi_{\rm phase}$ diverges like $(T - T_c)^{-1/2}$, while at high temperatures

$$\xi_{\rm phase} \simeq \frac{3}{4} \frac{\xi_{\rm pair}}{\sqrt{\ln\left[\frac{6\,\pi^2}{(k_F\,\lambda_T)^3}\right]}} .$$

$\Longrightarrow$



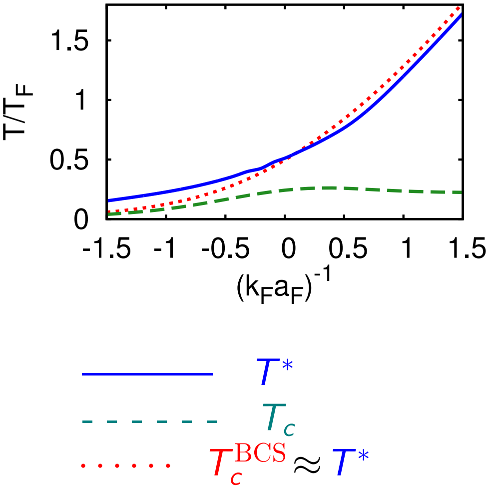
At any coupling, there exists a characteristic temperature T^* at which $\xi_{\text{pair}}(T)$ and $\xi_{\text{phase}}(T)$ cross each other.

Here are some examples:

Physical meaning of T^* :

T^* represents a *crossover temperature* below which independent pairs (whose partners are correlated over the length $\xi_{\rm pair}$) begin to build up mutual correlations over the length $\xi_{\rm phase}$ $\Longrightarrow$

precursor pairing phenomena occur below T^*



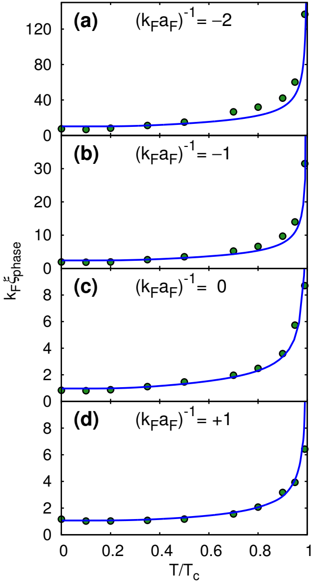
About a curiosity :

Temperature dependence of $\xi_{\rm phase}$ at the mean-field level below T_c, as obtained from:

- the present approach

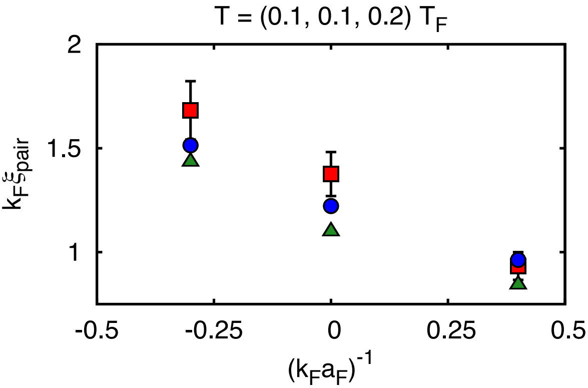
- the calculation of the profile of an isolated vortex in terms of the BdG equations (•)

[Simonucci *et. al.*, PRB **87**, 214507 (2013)].



Are we forgetting something ? Où est d'Artagnan ?

Where do $\xi_{\rm pair}$ and $\xi_{\rm phase}$ appear in the experimental data ?

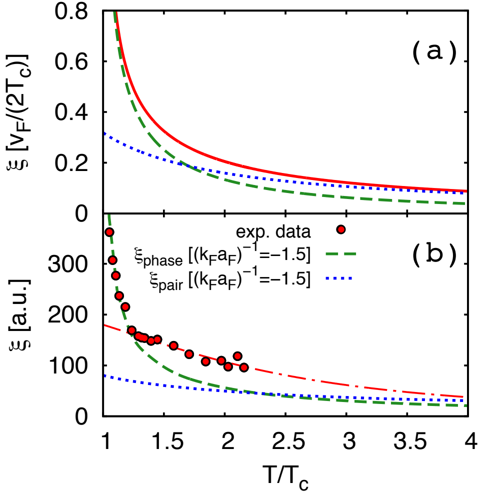


From RF spectra of ultra-cold Fermi gases ($T \ll T_c$):

exp. data (Ketterle) ■ $\Longrightarrow$ $\xi_{\rm pair}$

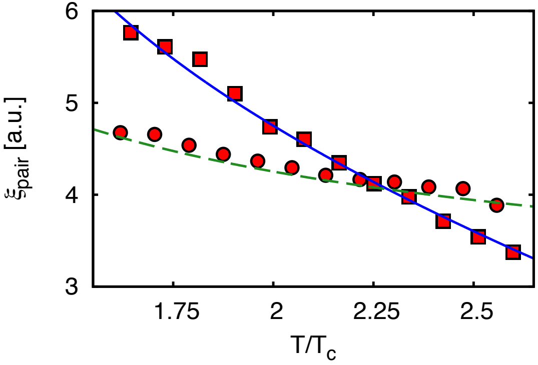
$T = 0$ mean field ▲

$+$ pairing fluct.s ●



(a) Temperature dependence of the length scale over which superconducting correlations survive in the normal phase [theory by Kogan, PRB **26**, 88 (1982) in the "extreme" BCS limit].

(b) Comparison with the data (•) by E. Polturak *et. al.*, PRL **67**, 3038 (1991) - proximity effect in an SS'S superconducting Josephson junction.



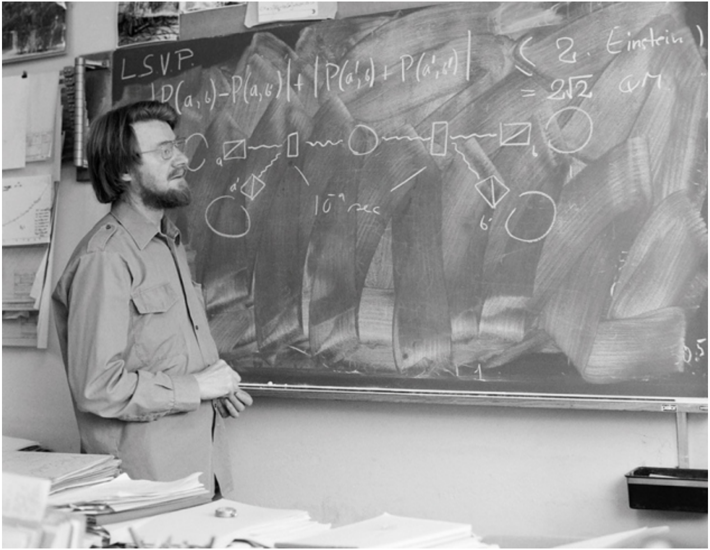
More recent data by Kirzhner & Koren (arXiv:1311.2250v1):

- for an optimally-doped (LSCO-0.18, ■) material
- for an under-doped (LSCO-0.10, •) material
- our calculation for $(k_F\, a_F)^{-1} = -3.0$

and for $(k_F\, a_F)^{-1} = -0.4$

And what about Cardinal Richelieu ?

Bell's equality [PRB **129**, 1896 (1963)]:



.. or interpreting a "sum rule" for $g_{\uparrow\downarrow}(\boldsymbol{\rho})$:

Quite generally, from the definition of $g_{\uparrow\downarrow}(\boldsymbol{\rho})$ one gets:

$$\int d\boldsymbol{\rho}\, g_{\uparrow\downarrow}(\boldsymbol{\rho}) = \frac{1}{V}\left(\langle N_\uparrow N_\downarrow\rangle - \langle N_\uparrow\rangle\langle N_\downarrow\rangle\right)$$

where $V =$ volume and $N_\sigma = \int d\mathbf{r}\, \psi^\dagger_\sigma(\mathbf{r})\psi_\sigma(\mathbf{r})$ $(\sigma = \uparrow, \downarrow)$.

On the other hand, for the "partial" compressibility one gets:

$$\left.\frac{\partial n_\uparrow}{\partial \mu_\downarrow}\right|_{T,V} = \frac{1}{V\, k_B T}\left(\langle N_\uparrow N_\downarrow\rangle - \langle N_\uparrow\rangle\langle N_\downarrow\rangle\right).$$

Comparison between the two expressions yields:

$$\boxed{\int d\boldsymbol{\rho}\, g_{\uparrow\downarrow}(\boldsymbol{\rho}) = k_B T\, \left.\frac{\partial n_\uparrow}{\partial \mu_\downarrow}\right|_{T,V}}$$

where the limit $n_\uparrow \to n_\downarrow \to n/2$ is understood.

The contradiction pointed out by Bell is here apparent $\Longrightarrow$ the above identity would imply $\int d\rho\, g_{\uparrow\downarrow}(\rho) = 0$ for $T \to 0$.

It would also imply that $\langle N_\uparrow N_\downarrow\rangle - \langle N_\uparrow\rangle\langle N_\downarrow\rangle = 0 \quad \Longleftrightarrow$ signifying a complete suppression of particle fluctuations.

Way out $\Longrightarrow$ this "sum rule" is obeyed by a "conserving" diagrammatic approximation in the sense of Baym-Kadanoff, provided *this approximation is made directly on the integral* of $g_{\uparrow\downarrow}(\rho)$ and not on $g_{\uparrow\downarrow}(\rho)$ before performing the integration.

Non commutativity of the results $\Longleftrightarrow$ fluctuations of particle number evaluated in grand canonical ensemble ("*before*") or canonical ensemble ("*after*") $\Longrightarrow$ the issue becomes irrelevant at high temperatures when classical physics holds !

Bell's equality vs Baym & Kadanoff:

The pair correlation function $g_{\uparrow\downarrow}(\boldsymbol{\rho})$ is not a response function

$\Longrightarrow$ it is not bound to satisfy conservation criteria *a la* Baym & Kadanoff.

Quite generally, to make connections with response functions one needs to introduce a "time variable" into the game.

This can be readily achieved by integrating $g_{\uparrow\downarrow}(\boldsymbol{\rho})$ over $\boldsymbol{\rho}$:

$$\int d\boldsymbol{\rho}\, g_{\uparrow\downarrow}(\boldsymbol{\rho}) + V\, n_{\uparrow} n_{\downarrow} = \frac{1}{V}\langle N_{\uparrow} N_{\downarrow}\rangle \qquad (\text{with } \beta = (k_B T)^{-1})$$

$$= \frac{1}{V\,\beta}\int_0^{\beta} d\tau\, \langle T_{\tau}\Big[\Big(e^{K\tau} N_{\uparrow} e^{-K\tau}\Big)\, N_{\downarrow}\Big]\rangle \qquad (\text{here is the crucial step !!})$$

$$= -\frac{1}{\beta}\int_0^{\beta} d\tau \int d\boldsymbol{\rho}\, \langle T_{\tau}\Big[\Psi_1(\boldsymbol{\rho},\tau)\Psi_2(\mathbf{0},0^+)\Psi_2^{\dagger}(\mathbf{0},0)\Psi_1^{\dagger}(\boldsymbol{\rho},\tau^+)\Big]\rangle$$

$$= -\frac{1}{\beta}\int_0^{\beta} d\tau \int d\boldsymbol{\rho}\, \mathcal{G}_2(\boldsymbol{\rho}\tau 1, \mathbf{0}0^+ 2; \boldsymbol{\rho}\tau^+ 1, \mathbf{0}02)$$

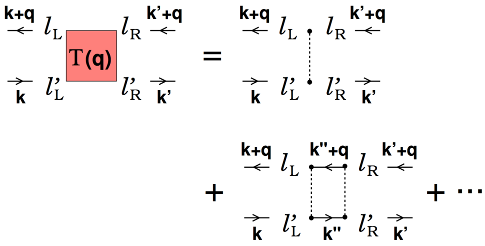
since N_{σ} *commutes with the grand-canonical Hamiltonian K* $= H - \mu_{\uparrow} N_{\uparrow} - \mu_{\downarrow} N_{\downarrow}$ while the density $\psi_{\sigma}^{\dagger}(\mathbf{r})\psi_{\sigma}(\mathbf{r})$ does not !

Here, the two-particle Green's function (in the Nambu's representation) $\mathcal{G}_2(1,2;1',2') = \langle T_\tau[\Psi(1)\Psi(2)\Psi^\dagger(2')\Psi^\dagger(1')]\rangle$ can be expressed in terms of the Bethe-Salpeter equation:

$$\mathcal{G}_2(1,2;1',2') = \mathcal{G}(1,1')\,\mathcal{G}(2,2') - \mathcal{G}(1,2')\,\mathcal{G}(2,1')$$
$$- \int d3456\,\mathcal{G}(1,3)\,\mathcal{G}(6,1')\;T(3,5;6,4)\,\mathcal{G}(4,2')\,\mathcal{G}(2,5)$$

to which criteria of "conserving" approximations apply.

As an example, let's consider the series of ladder diagrams for the many-particle T-matrix $\Longleftrightarrow$ the "extended" BCS (or RPA) approximation, which is familiar in the context of gauge invariance for the response of a BCS superconductor to an external electromagnetic field (P. Anderson):



After a (long but) straightforward calculation, one obtains:

$$\beta \int d\boldsymbol{\rho}\, g_{\uparrow\downarrow}(\boldsymbol{\rho})$$

$$= \int dk\, \mathcal{G}_{12}(k)^2 - \int dk \mathcal{G}_{11}(k)\mathcal{G}_{12}(k) \int dk' \mathcal{G}_{22}(k')\mathcal{G}_{21}(k') \frac{1}{\left[\int dk'' \mathcal{G}_{12}(k'')^2\right]^2}$$

where $\mathcal{G}_{11}$and $\mathcal{G}_{11}$are normal and anomalous single-particle BCS Green's functions, and

$$\int dk = \int \frac{d\mathbf{k}}{(2\pi)^3}\, k_B T \sum_n$$

On the other hand, at the level of BCS mean field (with a slight imbalance of spin populations) one obtains for $\left.\frac{\partial n_\uparrow}{\partial \mu_\downarrow}\right|_{T,V}$:

$$\frac{\partial n_\uparrow}{\partial \mu_\downarrow} = \left.\frac{\partial n_\uparrow}{\partial \mu_\downarrow}\right|_{\Delta} + \left.\frac{\partial n_\uparrow}{\partial \Delta}\right|_{\mu_\uparrow,\mu_\downarrow} \frac{\partial \Delta}{\partial \mu_\downarrow}$$

$$= \int dk\, \mathcal{G}_{12}(k)^2 - \frac{\int dk\, \mathcal{G}_{11}(k)\, \mathcal{G}_{12}(k)\ \int dk'\, \mathcal{G}_{22}(k')\, \mathcal{G}_{21}(k')}{\int dk''\, \mathcal{G}_{12}(k'')^2}$$

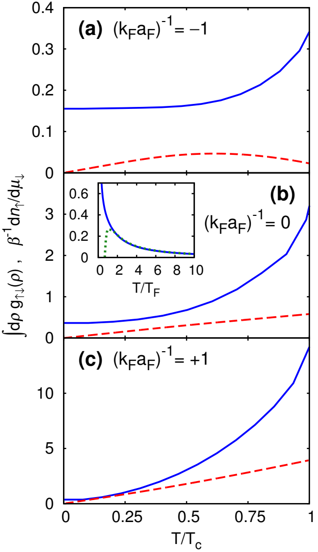
$\Longrightarrow$ comparison between these two expressions shows that the Bell's equality is satisfied at this level of a (conserving) approximation.

With the opposite procedure, of first approximating (the Bethe-Salpeter equation for) $g_{\uparrow\downarrow}(\boldsymbol{\rho})$ by the extended BCS (or RPA) approximation and *then* integrating it over $\boldsymbol{\rho}$, marked deviations result from the values of $\frac{1}{\beta} \left. \frac{\partial n_\uparrow}{\partial \mu_\downarrow} \right|_{T,V}$.

Here are some examples of their different temperature dependence for various couplings below T_c:

$\int d\boldsymbol{\rho}\, g_{\uparrow\downarrow}(\boldsymbol{\rho})$

$\frac{1}{\beta} \left. \frac{\partial n_\uparrow}{\partial \mu_\downarrow} \right|_{T,V}$



The inset in the central panel shows a corresponding comparison made at unitarity in the high-temperature regime, where the (non-self consistent) t-matrix approximation becomes exact and classical physics takes over.

Conclusions :

- ♣ We have implemented the concept of the wave function of a Cooper pair at any temperature and coupling, distinguishing the "internal" from the "center-of-mass" wave function.
- ♣ We have presented a description in terms of a minimal diagrammatic structure which englobes these concepts in a unified way above T_c.
- ♣ We have given a well-defined physical meaning to the crossover temperature T^*, below which precursor pairing phenomena begin to show.
- ♣ Twenty years have not passed in vain !

Thank you for your attention !