Ab initio identification of the pseudogap phase in Fermi gas with large scattering length

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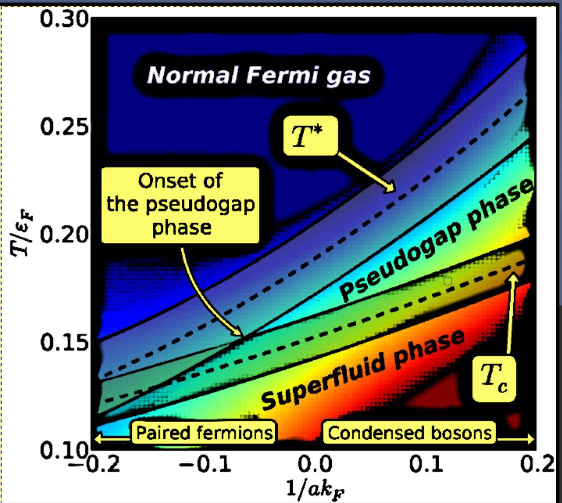
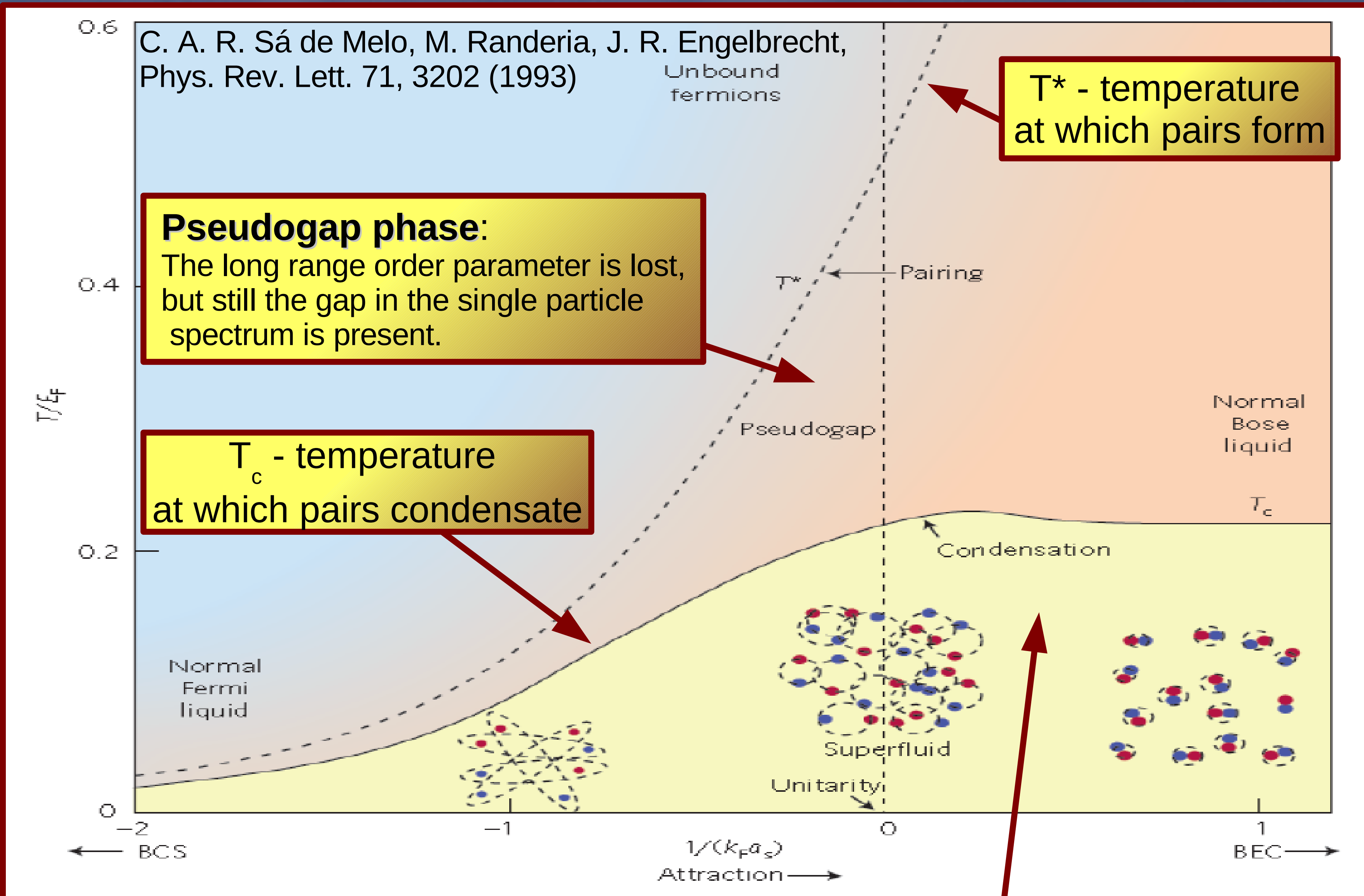


arXiv:1103.4382

Pseudogap phase - definition

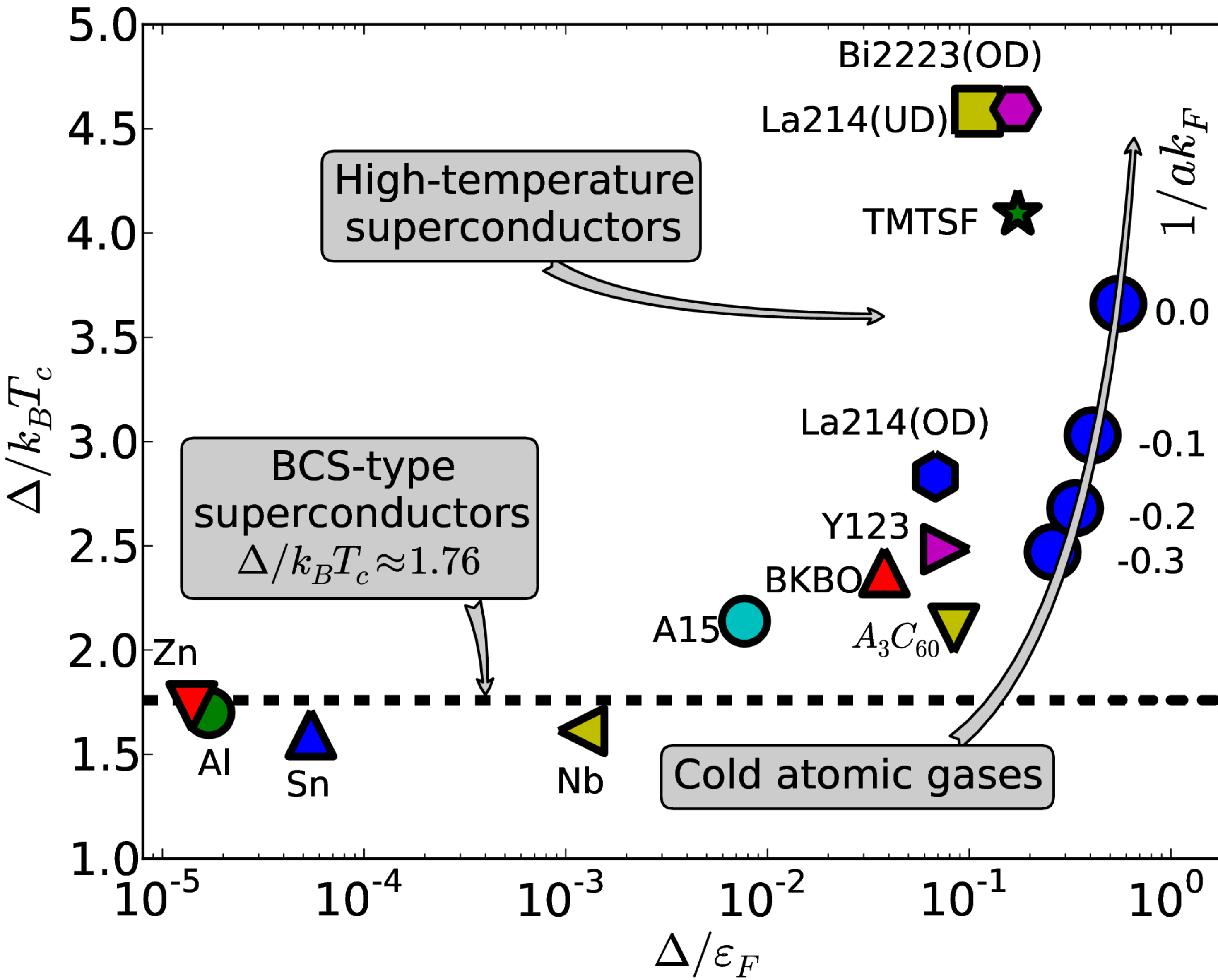


off-diagonal long-range order parameter

$$\lim_{r\to\infty}\int d^3\mathbf{r}_1 d^3\mathbf{r}_2 \langle\psi^\dagger_\uparrow(\mathbf{r}_1+\mathbf{r})\psi^\dagger_\downarrow(\mathbf{r}_2+\mathbf{r})\psi_\downarrow(\mathbf{r}_2)\psi_\uparrow(\mathbf{r}_1)\rangle \neq 0,$$

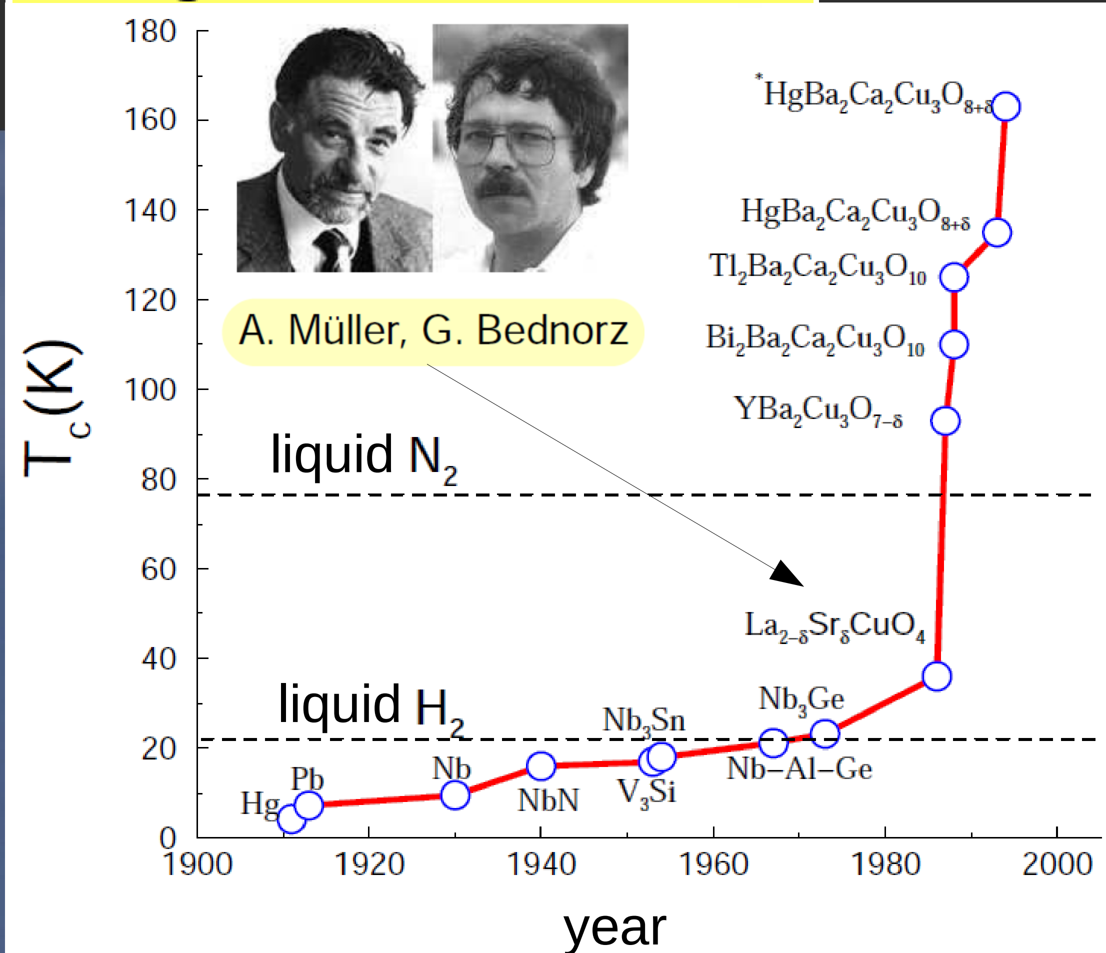
Pseudogap and HTSC

P. Magierski, G.W., A. Bulgac, arXiv:1103.4382



the highest Tc overall is 18 C

Pseudogap and HTSC

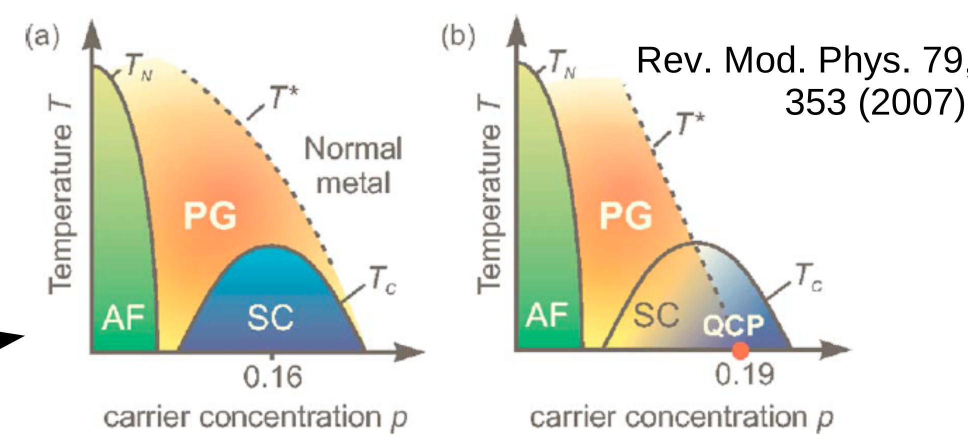


Two main mechanisms which could be responsible for the appearance of pseudogap phase in HTSC:

(a): pairing precursor (the Cooper pair formation above T_c)

(b): two-particle correlations of different physical origin

Problems of interpretation of pseudogap state in HTSC (lattice structure, impurities).



Rev. Mod. Phys. 79, 353 (2007)

FIG. 34. (Color online) Two scenarios for the hole-doped HTS phase diagram. (a) T^* merges with T_c on the overdoped side. (b) T^* crosses the superconducting dome (SC) and falls to zero at a quantum critical point (QCP). T_N is the Néel temperature for the antiferromagnetic (AF) state.

Earlier studies

A. PERALI, P. PIERI, G. C. STRINATI, AND C. CASTELLANI
PHYSICAL REVIEW B **66**, 024510 (2002)

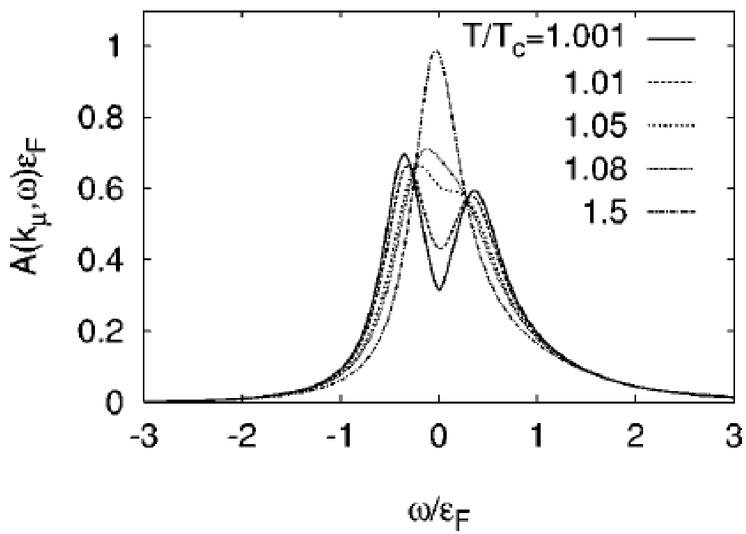
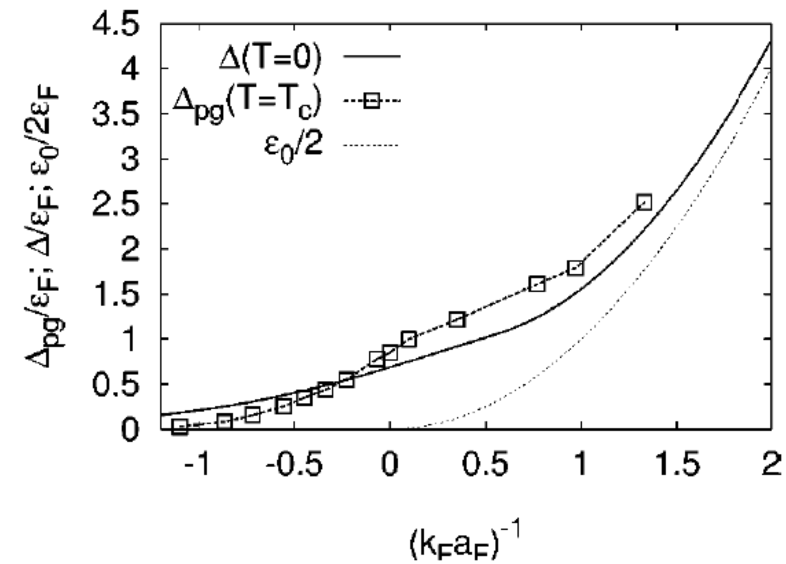
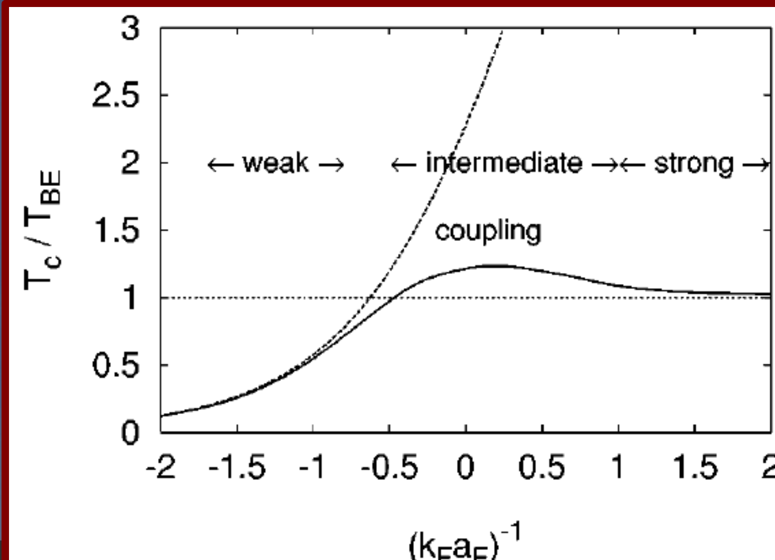


FIG. 13. Spectral function at $|\mathbf{k}|=k_\mu$, as a function of frequency (in units of ϵ_F) at different temperatures. In this case, with $(k_F a_F)^{-1}=-0.45$ $(T_c/\epsilon_F=0.23)$. (Intermediate- to weak-coupling regime.)

The diagrammatic scheme we consider is based on the non-self-consistent *t*-matrix approximation, constructed with "bare" single-particle Green's functions [with the inclusion, however, of the dressed chemical potential and of an additional constant energy shift (to be discussed below) which is relevant to the symmetry of the spectral function]. This

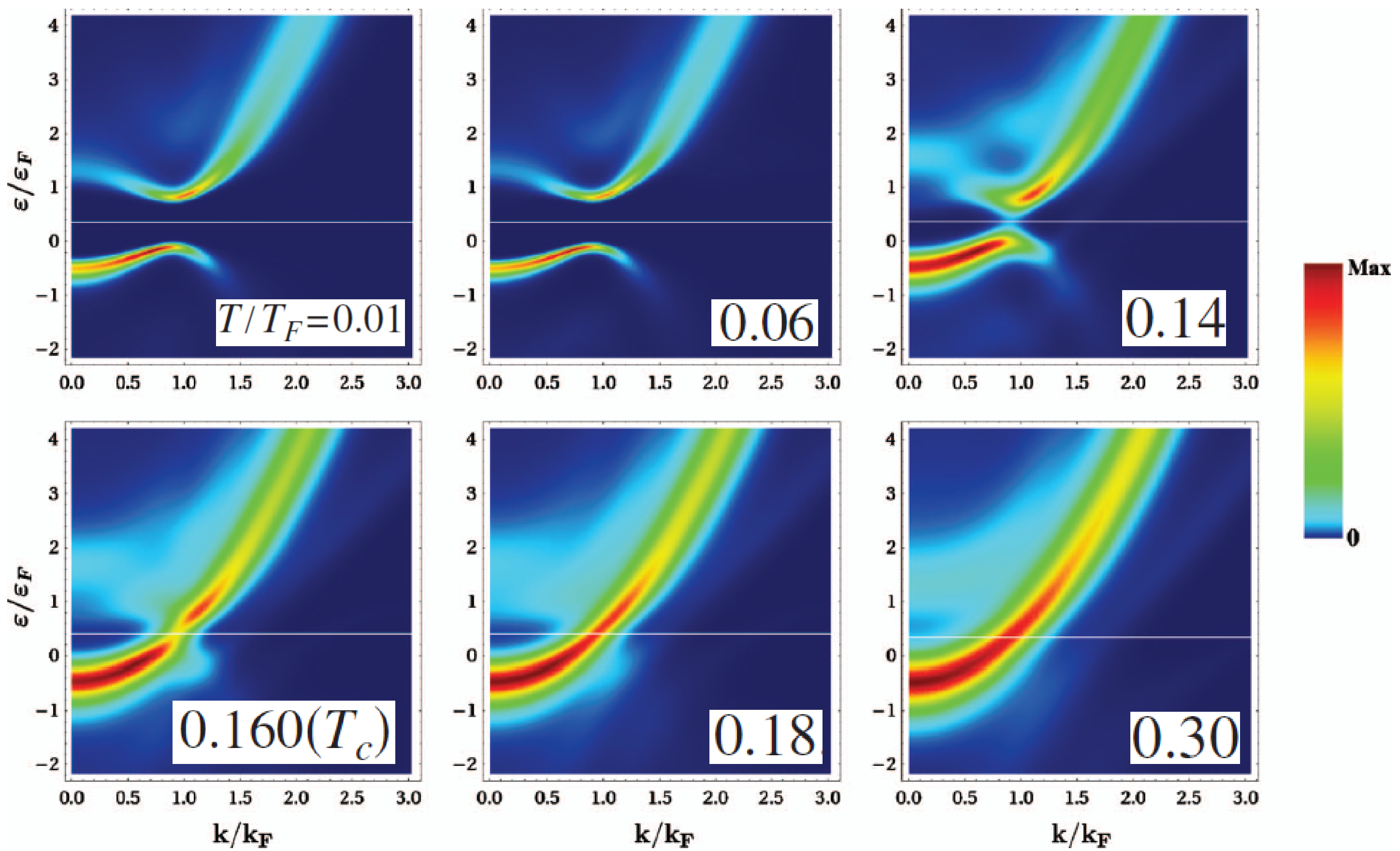




Earlier studies

Our calculation of the spectral functions for a dilute system of ultracold fermionic atoms is based on a Luttinger-Ward approach to the BCS-BEC crossover that has been presented in detail previously [21,26]. As a starting point, we

HAUSSMANN, PUNK, AND ZWERGER
PHYSICAL REVIEW A **80**, 063612 (2009)

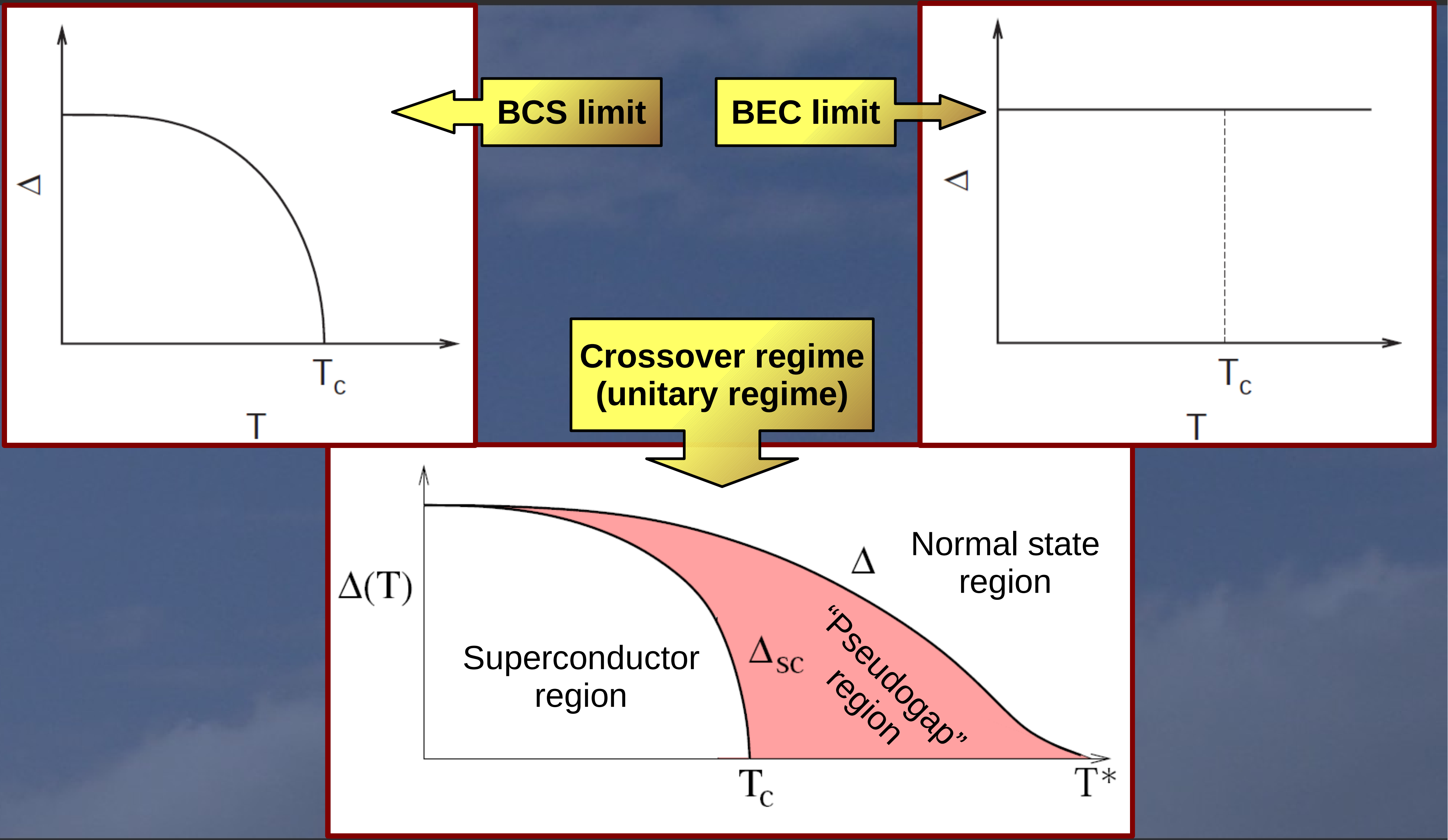


Different approaches
=
different results

Chih-Chun Chien,
Hao Guo,
Yan He, and K. Levin
Comparative study of BCS-BEC crossover theories above Tc.
Phys. Rev. A 81, 023622 (2010)

Finite temperature QMC calculations of the spectral function at unitarity by Bulgac *et al.* [67] indicate the presence of a gapped particle excitation spectrum of form (4.1) also above the critical temperature, which is not found in our approach. More generally, it is evident from the spectral

BCS–BEC crossover



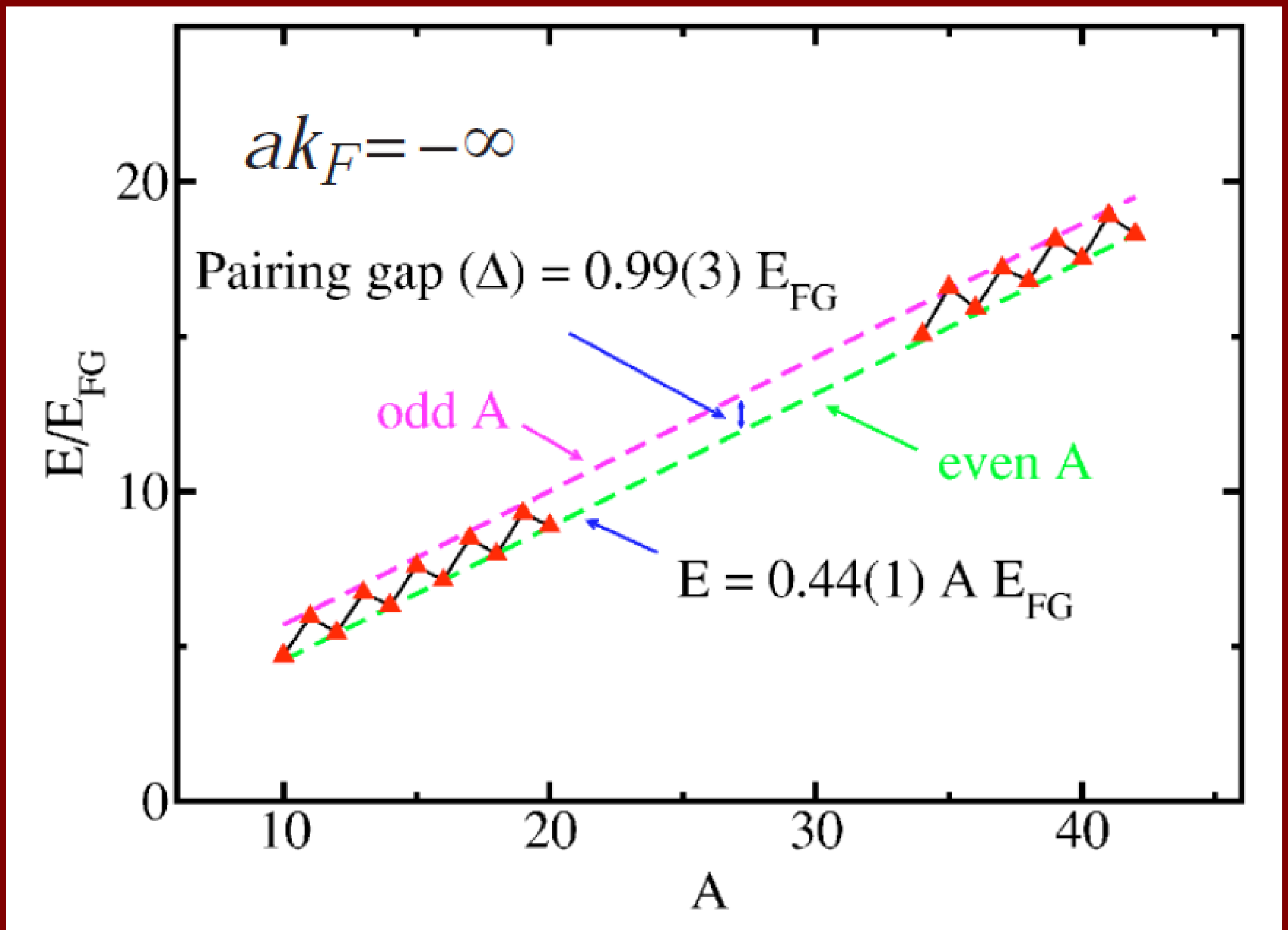
Pictures taken from: Q. Chen et al., Physics Reports 412 (2005) 1–88

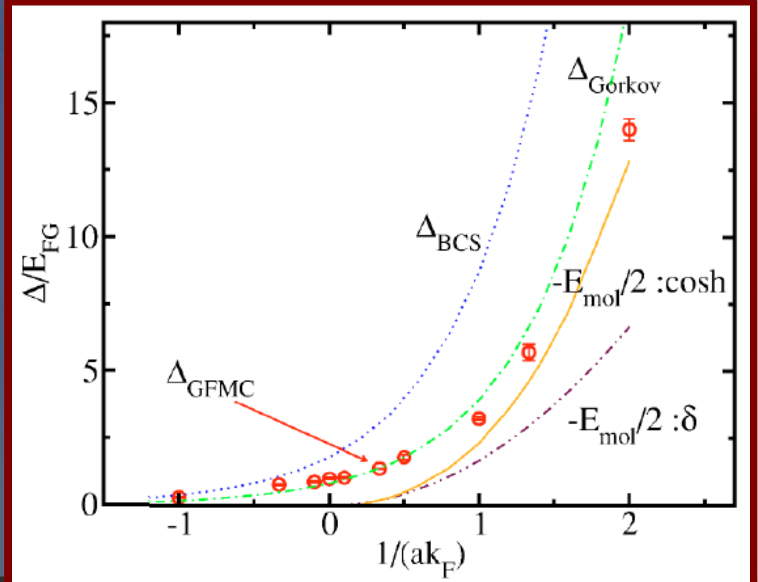
Computing the energy gap within QMC

Standard approach

$$\Delta(N = 2n + 1) = E(N) - \frac{1}{2}[E(N-1) + E(N+1)],$$

Good for zero temperature calculations





Carlson J., Chang S.-Y., Pandharipande V.R., Schmidt K.E., Phys. Rev. Lett. 91, 050401 (2003)

Computing the energy gap within QMC

Standard approach

$$\Delta(N = 2n + 1) = E(N) - \tfrac{1}{2}[E(N-1) + E(N+1)],$$

But QMC at finite temperatures require to use grand canonical ensemble

Particle number not fixed!

$$E(\beta,\mu) = \frac{1}{Z(\beta,\mu)} \mathrm{Tr}\left\{\hat{H}\exp[-\beta(\hat{H}-\mu\hat{N})]\right\},$$

$$Z(\beta,\mu) = \mathrm{Tr}\left\{\exp[-\beta(\hat{H}-\mu\hat{N})]\right\},$$

$$P_{N_0} = \delta(\hat{N} - N_0) = \int_0^{2\pi} d\alpha\, \exp[-i\alpha(\hat{N} - N_0)]$$

Projection on good particle number is required...

EXTREMELY TIME CONSUMING!

Spectral function

Alternative approach:
Spectral weight function (defines the spectrum of possible energies ω, for a particle with momentum **p** in the medium)

$$A_{\lambda\lambda'}(\mathbf{p},\omega) = \int d^3\mathbf{r} \int dt\; e^{-i(\mathbf{p}\cdot\mathbf{r}-\omega t)} \langle \{ \hat{\psi}_\lambda(\mathbf{r},t), \hat{\psi}^\dagger_{\lambda'}(\mathbf{0},0) \} \rangle .$$

BCS theory gives:

$$A(\boldsymbol{p},\omega) = 2\pi\,|u_{\boldsymbol{p}}|^2\,\delta(\omega - E(\boldsymbol{p})) + 2\pi\,|v_{\boldsymbol{p}}|^2(\boldsymbol{p})\,\delta(\omega + E(\boldsymbol{p}))$$

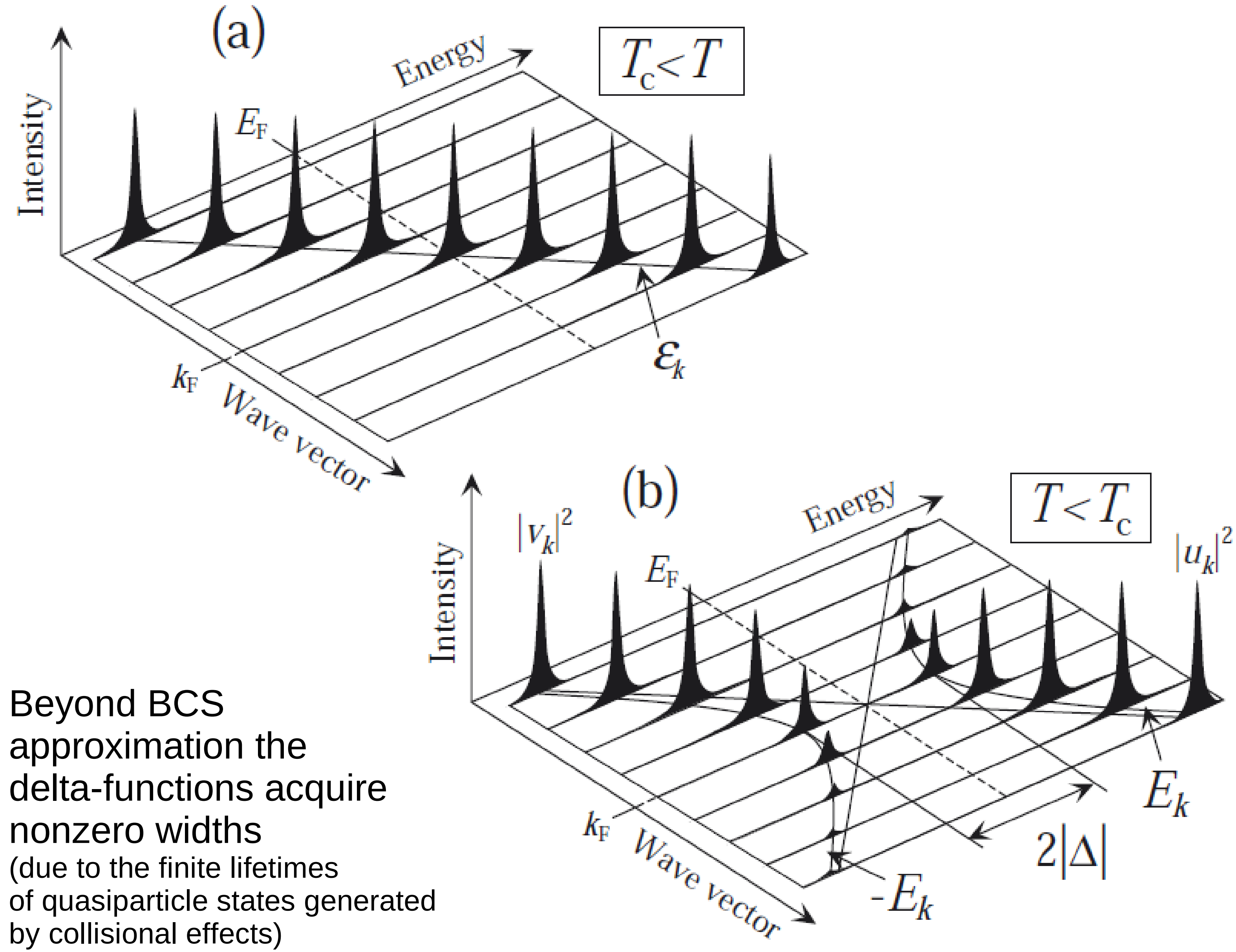
$$E(\boldsymbol{p}) = \sqrt{\left(\frac{p^2}{2m^*} + U - \mu\right)^2 + \Delta^2},$$

"pairing" gap

Effective mass

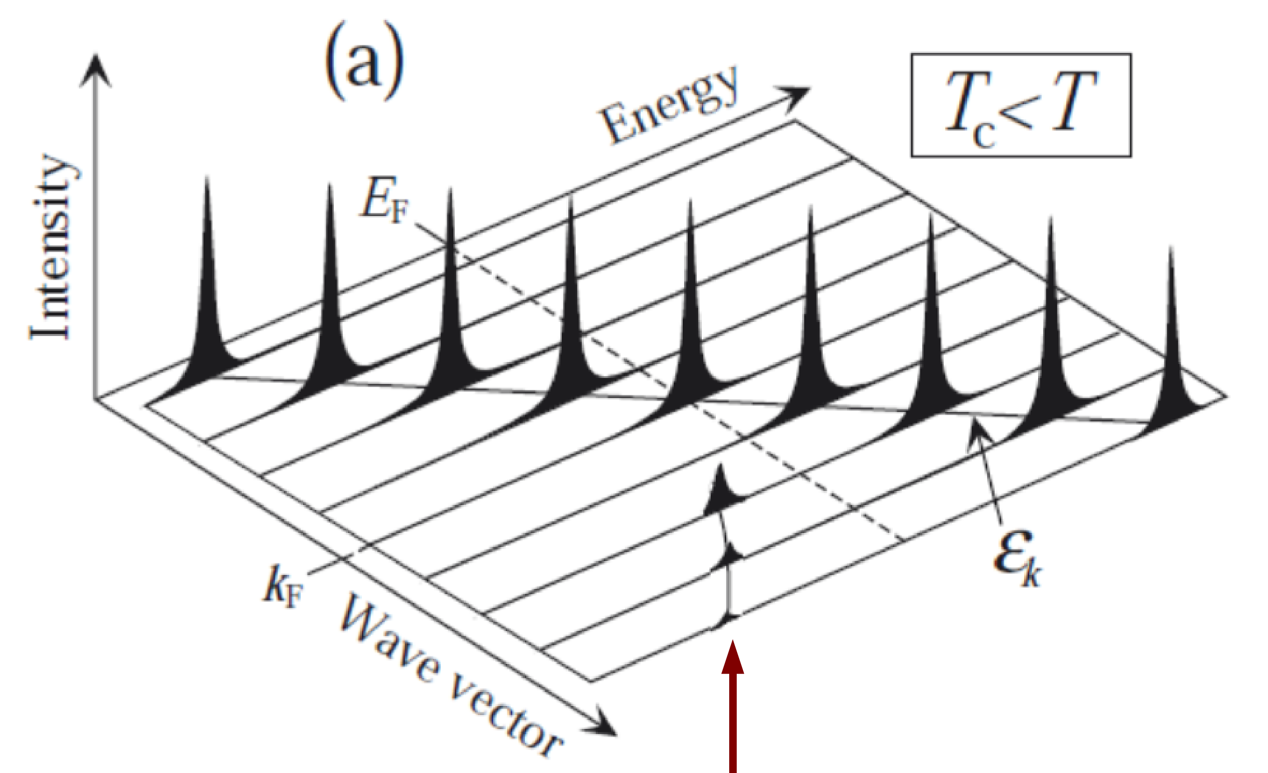
Self energy

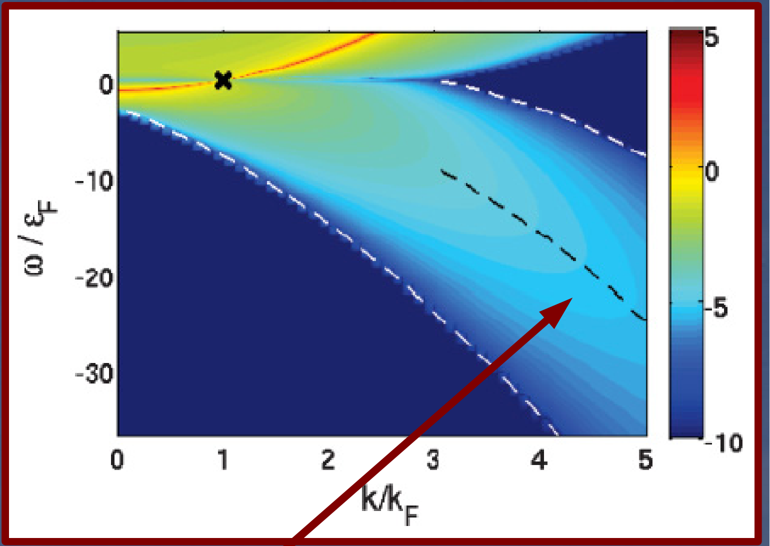
Spectral function – BCS case



Beyond BCS approximation the delta-functions acquire nonzero widths
(due to the finite lifetimes of quasiparticle states generated by collisional effects)

Spectral function of dilute Fermi gases





Conclusions. We have shown that there is an unusual feature in the large-momentum structure of the single-particle spectral function of *all* dilute Fermi gases, normal or superfluid, which is closely related to the universal short-distance features discussed by Tan and others [9,10]. This is an incoherent branch of the dispersion, where ω goes like *negative* $\epsilon_{\mathbf{k}}$ [28],

W.Schneider and M.Randeria, Phys. Rev. A 81, 021601(R) (2010)

Computing the spectral function within QMC

$$A_{\lambda\lambda'}(\mathbf{p},\omega) = \int d^3\mathbf{r} \int dt\; e^{-i(\mathbf{p}\cdot\mathbf{r}-\omega t)} \langle\{\hat{\psi}_\lambda(\mathbf{r},t), \hat{\psi}^\dagger_{\lambda'}(\mathbf{0},0)\}\rangle.$$

$$\mathcal{G}_{\lambda\lambda'}(\mathbf{r}t,\mathbf{r}'t') = -i\langle\mathcal{T}_t[\hat{\psi}_\lambda(\mathbf{r}t)\hat{\psi}^\dagger_{\lambda'}(\mathbf{r}'t')]\rangle,$$

Close connection with real time propagator

But QMC can only provide one-body temperature Green's (Matsubara) function

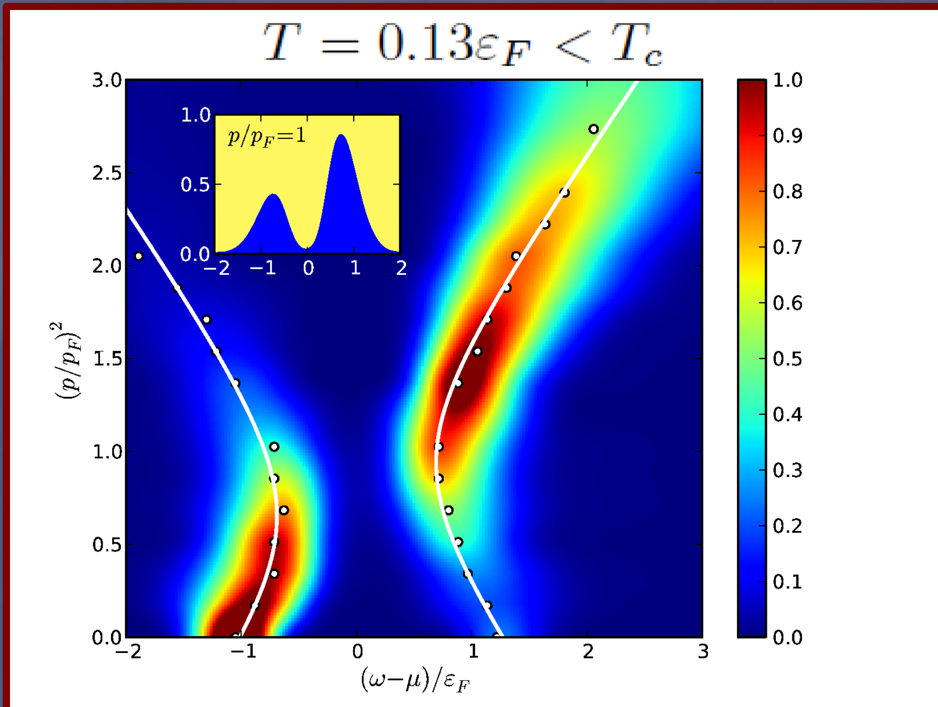
$$\mathcal{G}(\boldsymbol{p},\tau) = \frac{1}{Z}\mathrm{Tr}\{\exp[-(\beta-\tau)(H-\mu N)]\psi^\dagger(\boldsymbol{p}) \times \exp[-\tau(H-\mu N)\psi(\boldsymbol{p})]\},$$

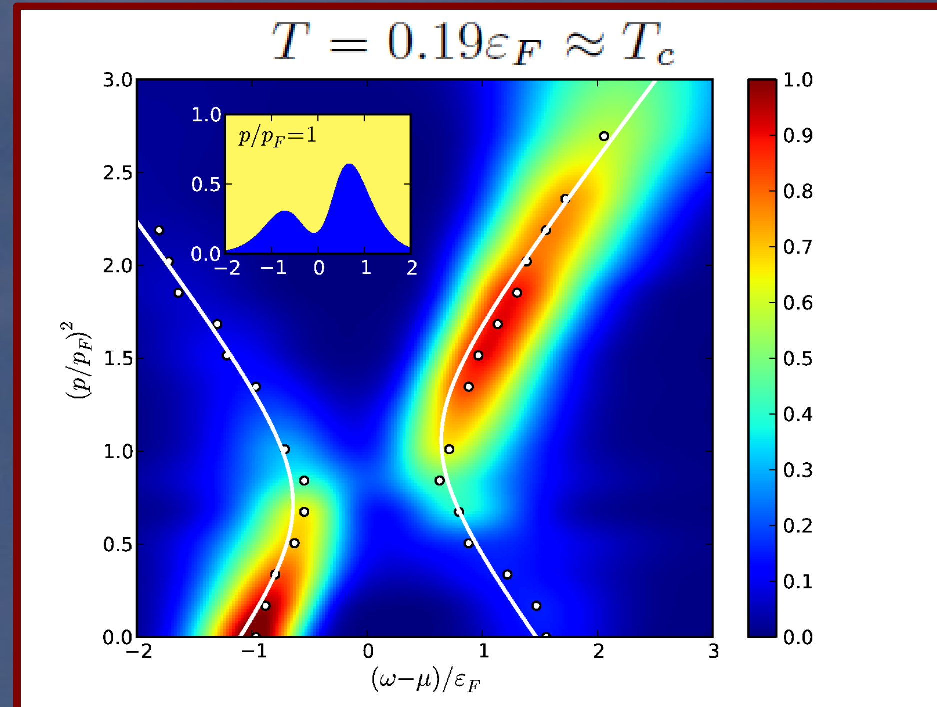
Analytic continuation of the imaginary time propagator to real frequencies is required.

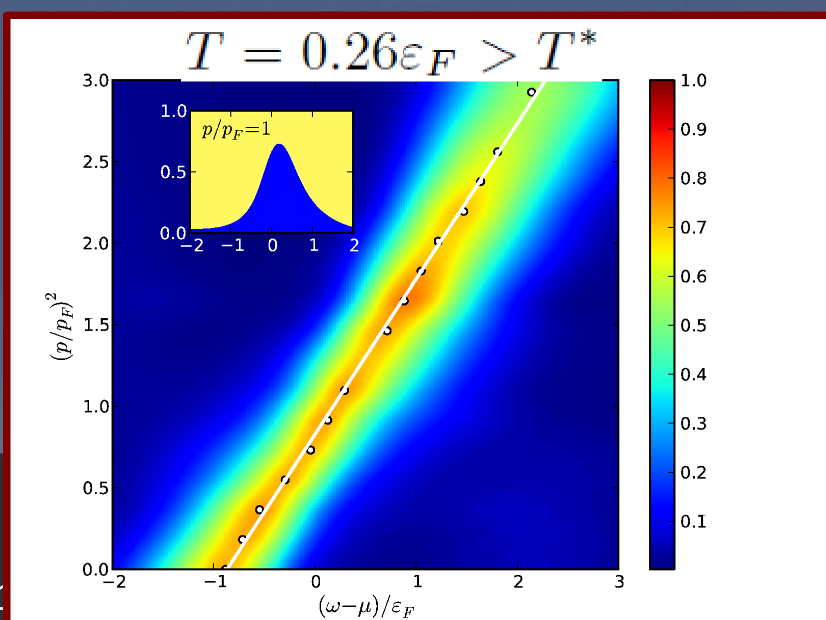
$$\mathcal{G}(\boldsymbol{p},\tau) = -\frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega A(\boldsymbol{p},\omega)\frac{\exp(-\omega\tau)}{1+\exp(-\omega\beta)}.$$

The problem is ill-posed!
We used (simultaneously):
***Maximum Entropy Method* and**
Singular Value Decomposition
Method

Spectral weight function for 1/ak$_F$=0.2 (BEC side)

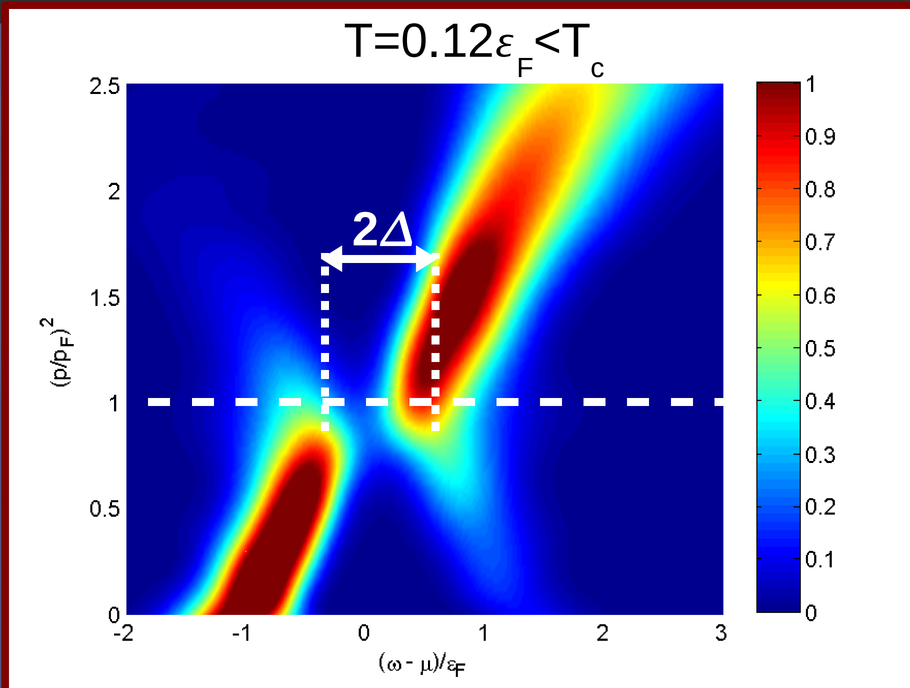


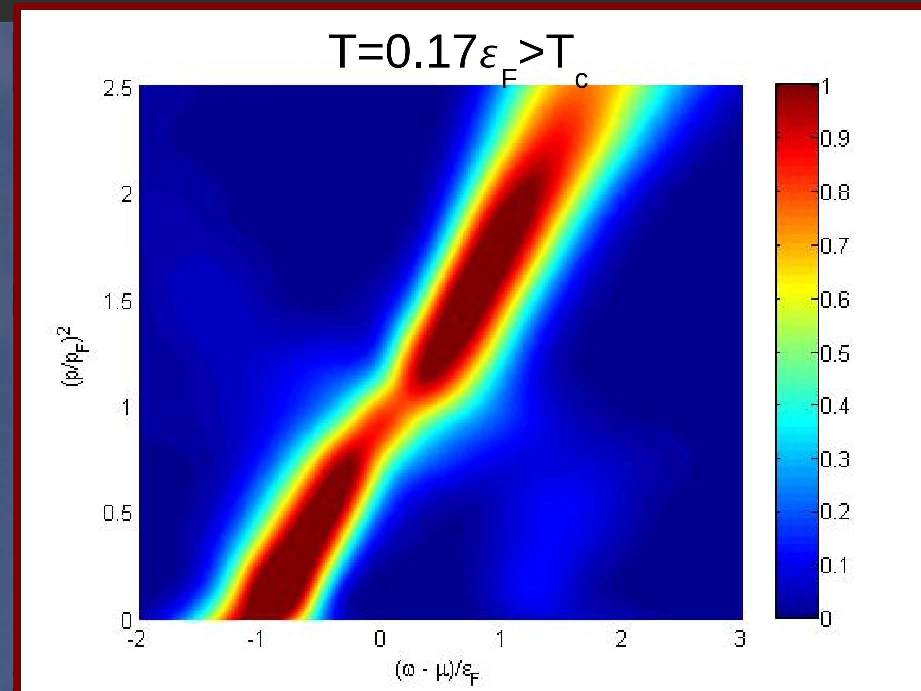


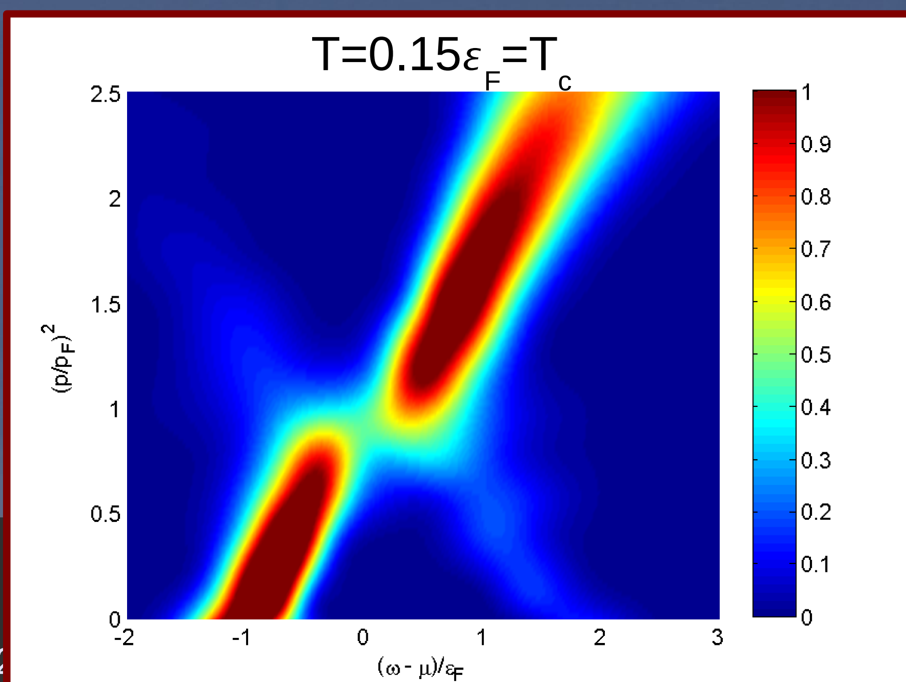


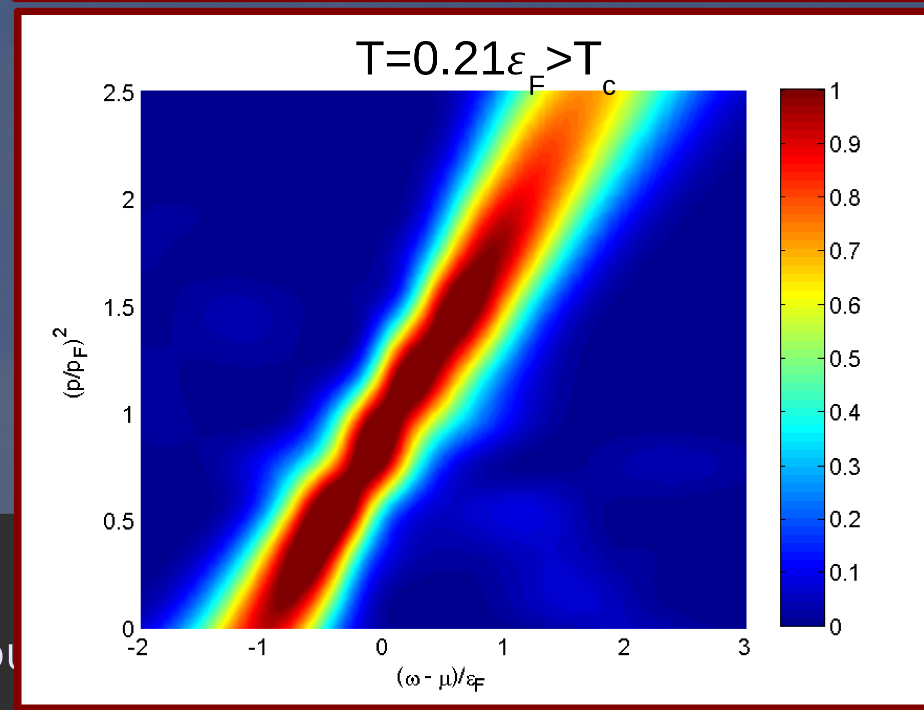
Technical details:
* lattice: 10^3
* number of particles: ~100
* statistical errors of imaginary time propagator: below 1%
* systematic errors: do not exceed 10%

Spectral weight function for unitary limit









Analytic continuation - limitation

$$\mathcal{G}_i \;\; (i = 1, 2, \ldots, \mathcal{N}_\tau)$$

$$\mathcal{G}_i = \int_{-\infty}^{+\infty} d\omega\, \phi_i^*(\omega) A(\omega)$$

$$\phi_i(\omega) = -\frac{1}{2\pi} \frac{e^{-\omega\tau_i}}{1+e^{-\omega\beta}}$$

If ϕ_i are not linearly independent then linear inverse problem is ill-posed.

The solution can be divided into two parts:

$$A(\omega) \;=\; A^\dagger(\omega) + A_\perp(\omega),$$

Invisible part

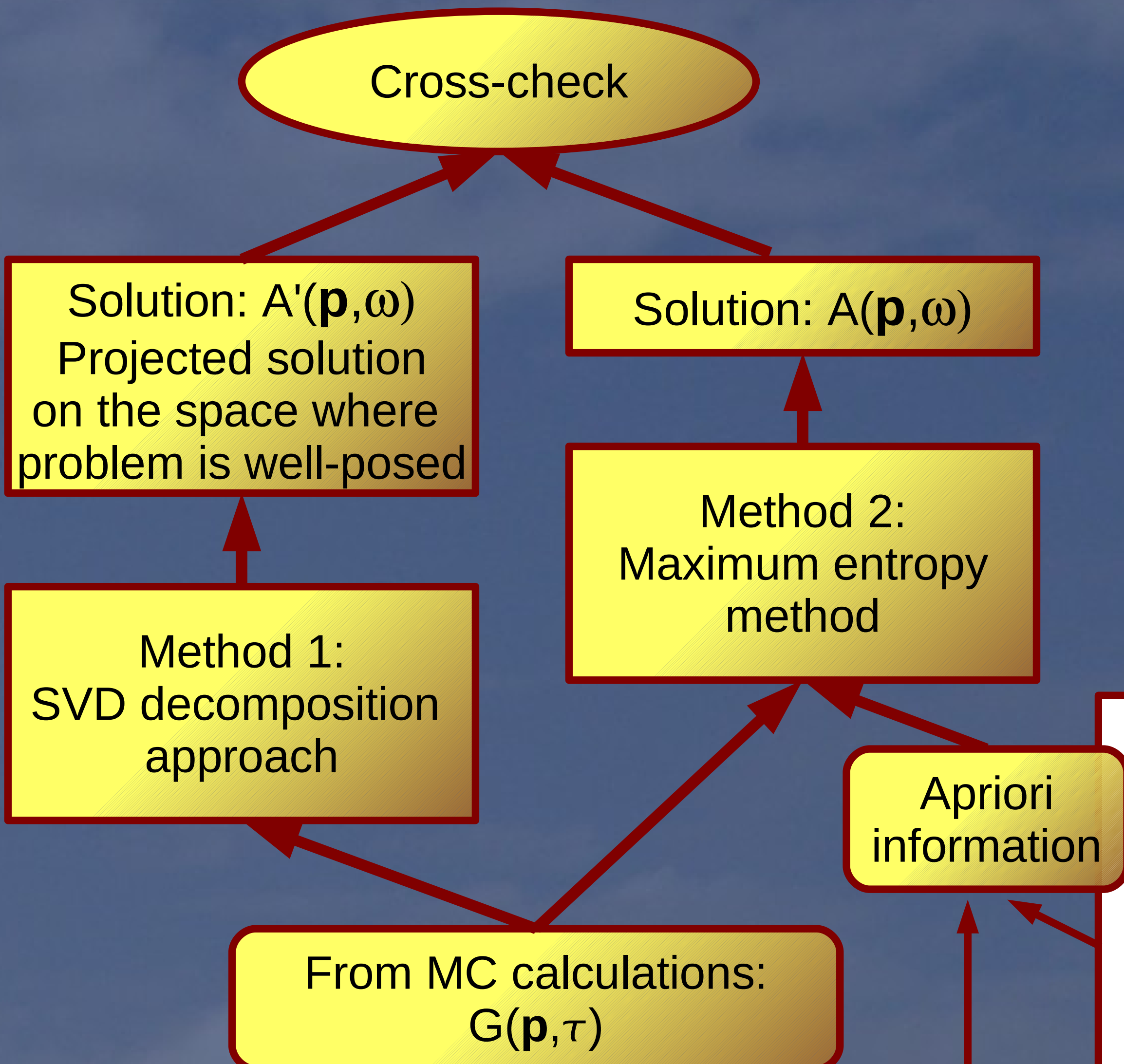
Normal solution fully determined by data G_i

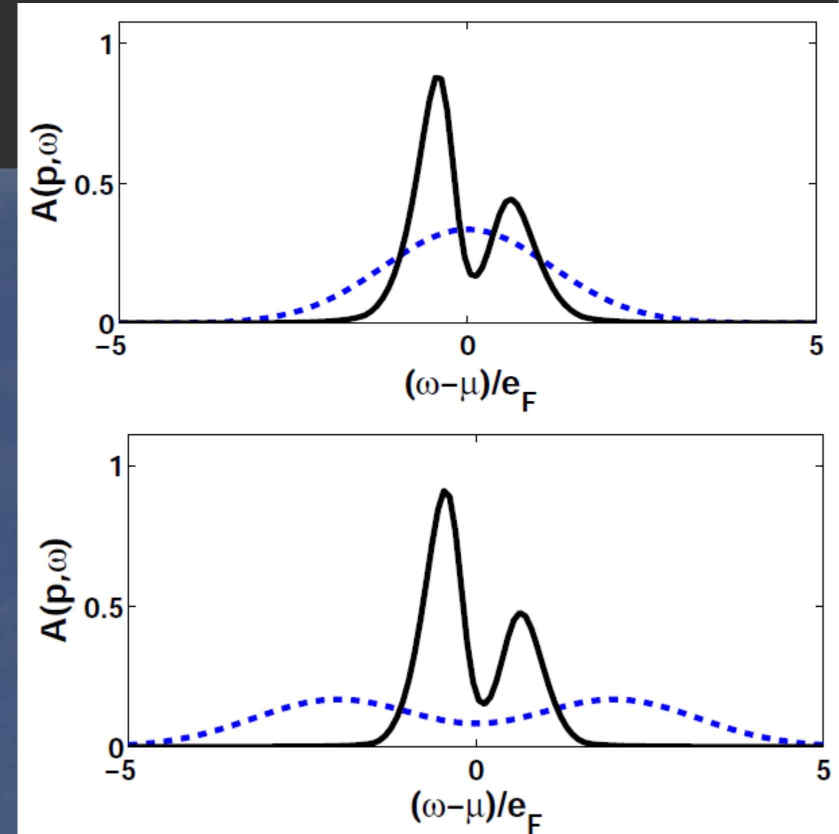
SVD Method

A priori information to “fix” invisible part

Maximum Entropy Method

Methodology





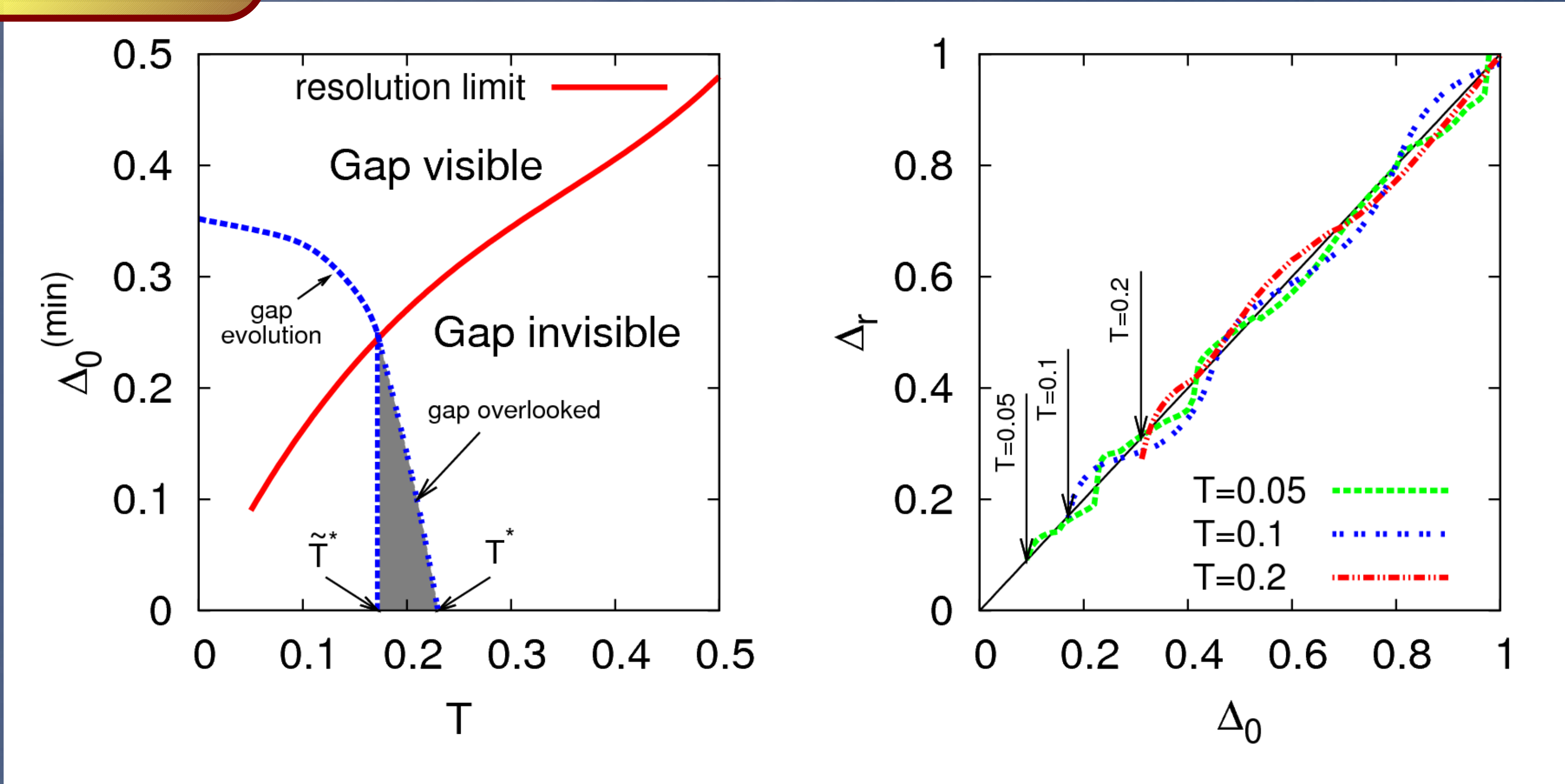
$$A(\mathbf{p},\omega) \geqslant 0, \qquad \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} A(\mathbf{p},\omega) = 1,$$

$$\int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} A(\mathbf{p},\omega) \frac{1}{1+\exp(\omega\beta)} = n(\mathbf{p}),$$

Gaussian-like structure for $A(\mathbf{p},\omega)$

Analytic continuation - limitation

Artificial spectral function with gap Δ_0 ⇒ $A \Rightarrow G_i$ ⇒ Adding noise to G_i ⇒ Reconstruction $G_i \Rightarrow A$ ⇒ Extracting gap Δ_r

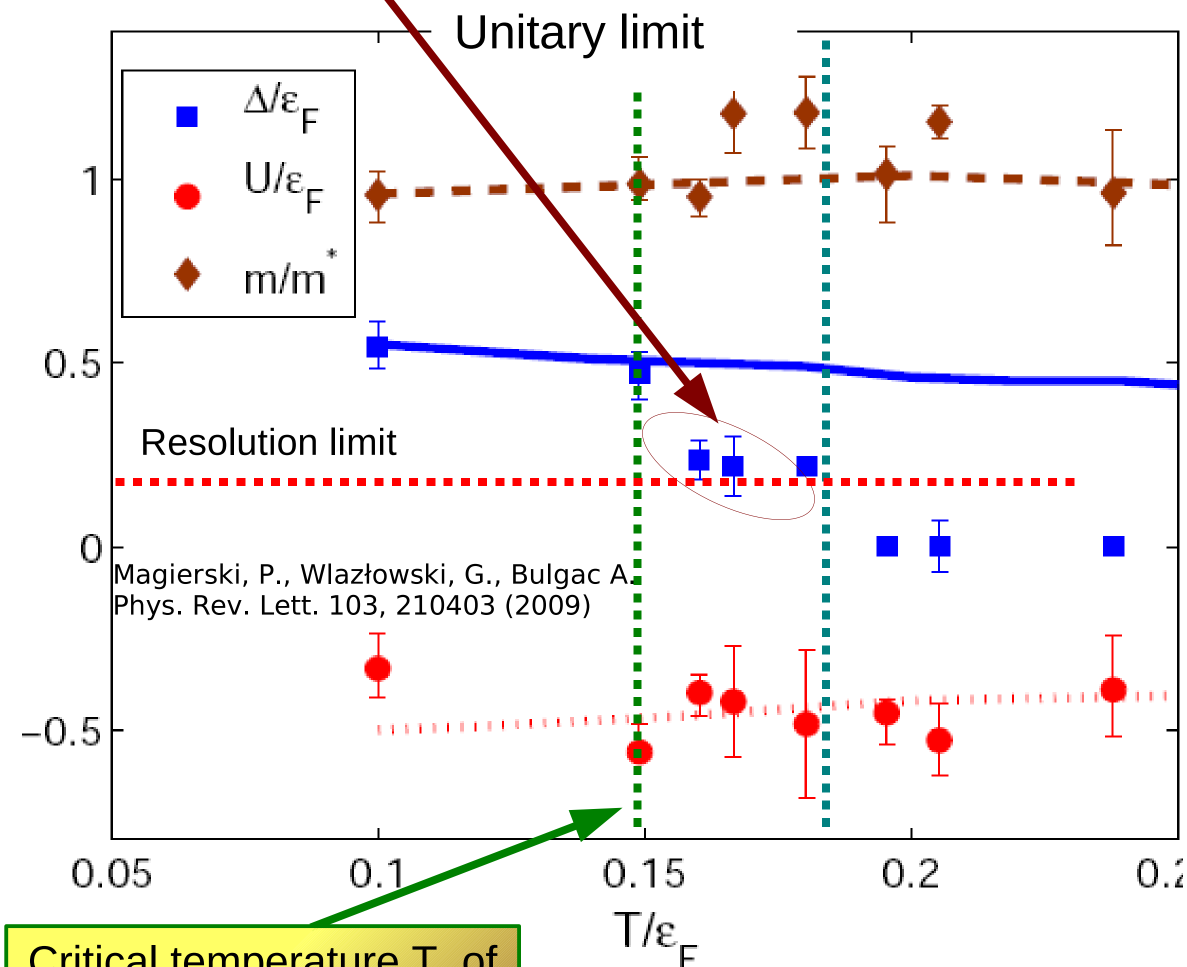


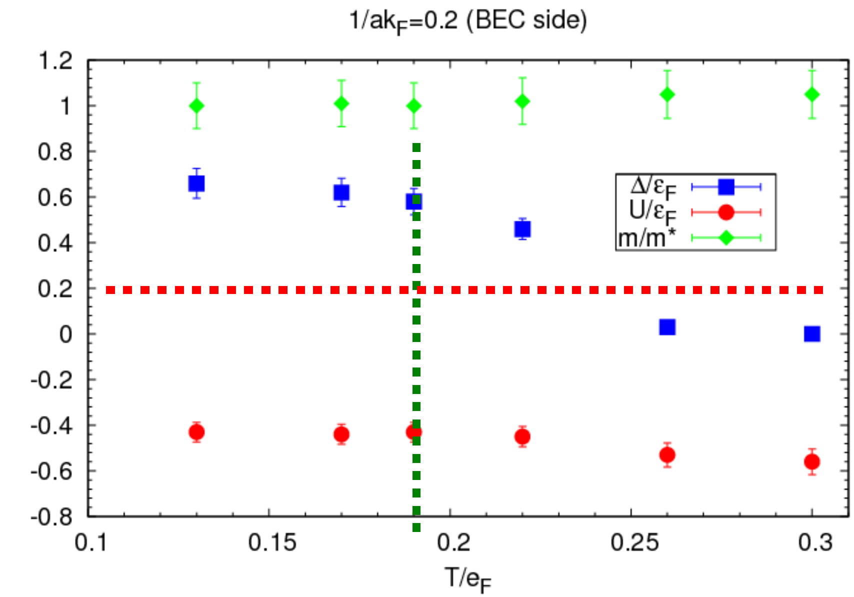
If size of the energy gap is smaller than *resolution limit* one cannot distinguish between the spectral weight function with and without energy gap.

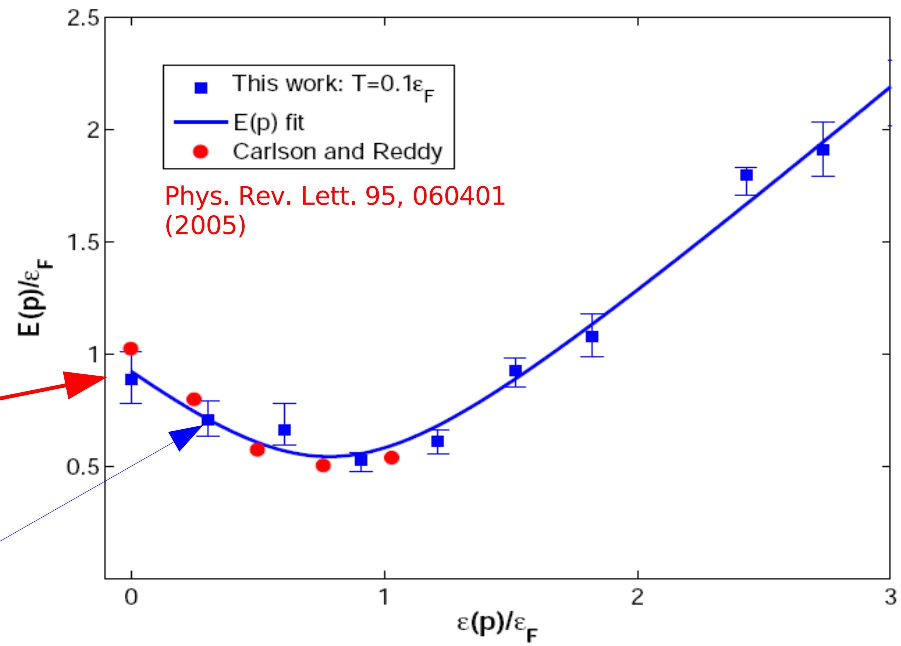
The approach can only provide a lower bound for the gap vanishing temperature.

Energy gap for unitary limit

The energy gap exists above the critical temperature!





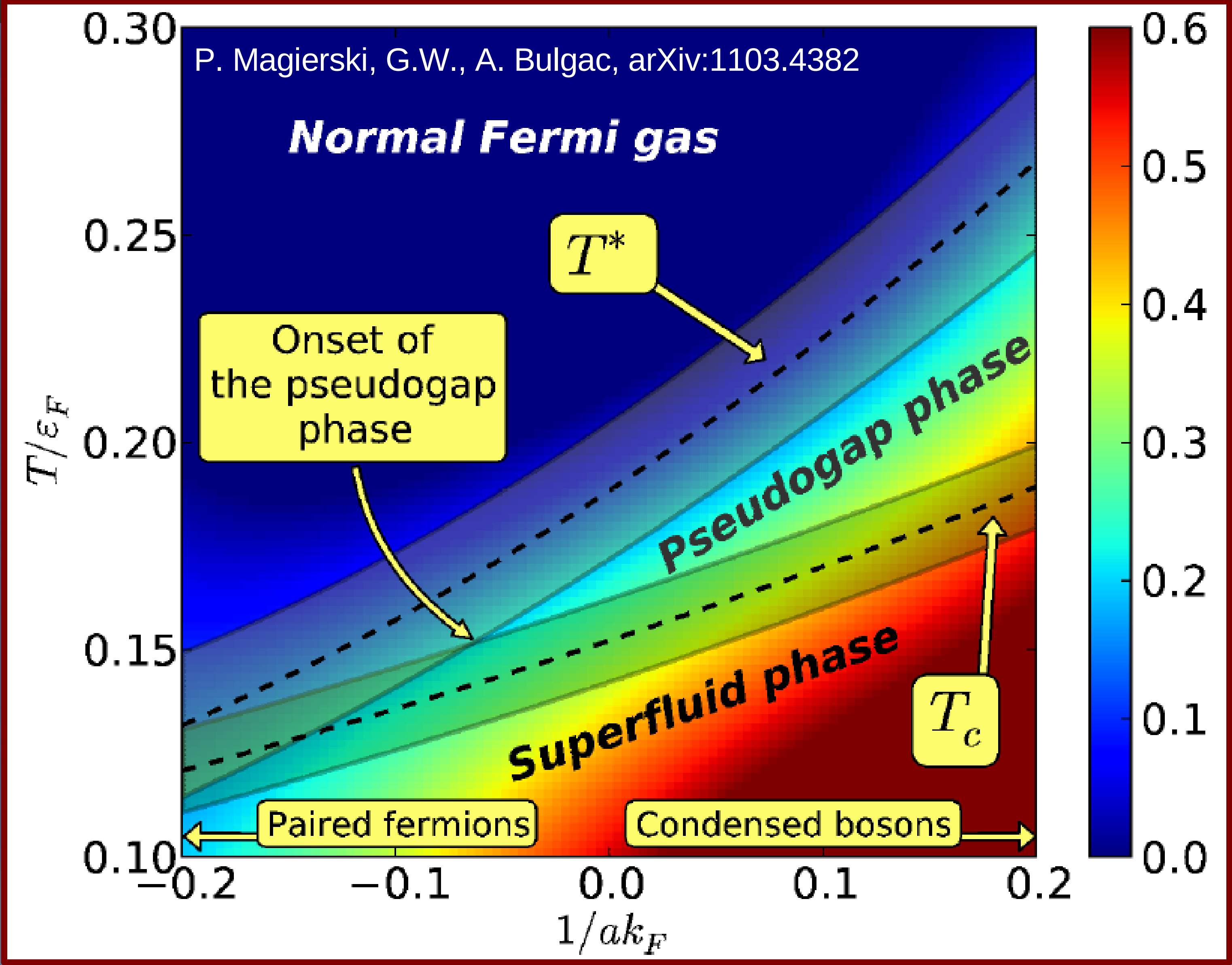


Critical temperature T_c of the superfluid-normal phase transition

Fix node MC calculations at T=0

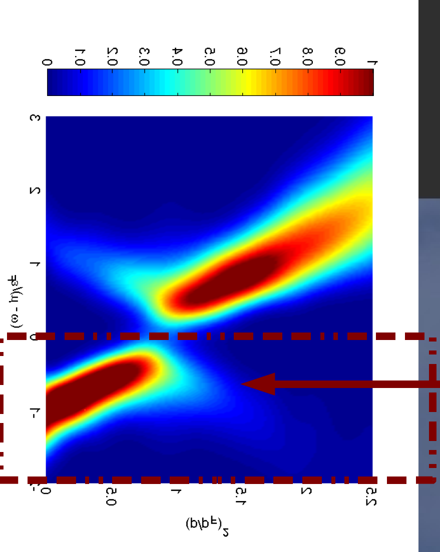
Quasiparticle spectrum extracted from the spectral function at $T=0.1e_F$

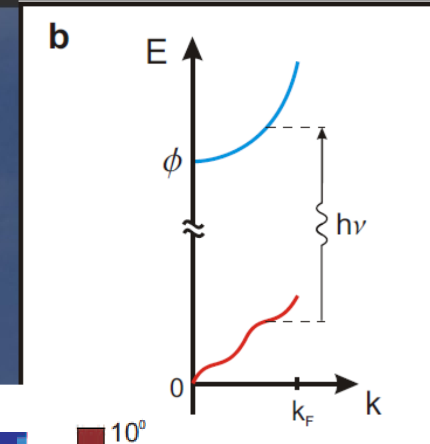
Evolution of the energy gap



***Ab initio* result: The onset of pseudogap phase at $1/ak_F \approx -0.05$.**

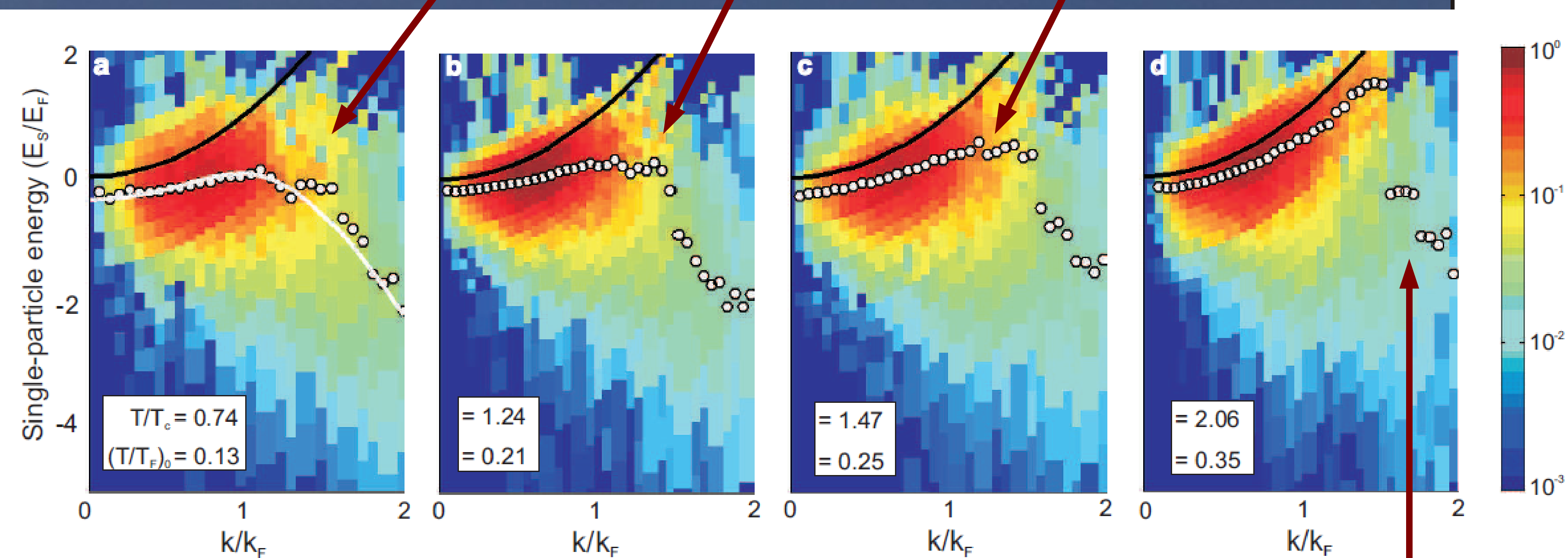
Momentum-resolved rf spectroscopy





Only occupied branch accessible.

The "back-bending" structure around the Fermi momentum is related with energy gap



Results for 1/akF=0.15 (BEC side)

universal behavior that gives rise to a weak, negatively dispersing feature

Gaebler, J.P., Stewart, J.T., Drake, T.E., Jin, D.S., Perali, A., Pieri, P. & Strinati, Nature Physics 6, 569 (2010)

Momentum-resolved rf spectroscopy

Since the experiments with cold atoms are performed in a trap one has to translate the results obtained for the uniform system to the nonuniform one determined by the geometry of a trap.

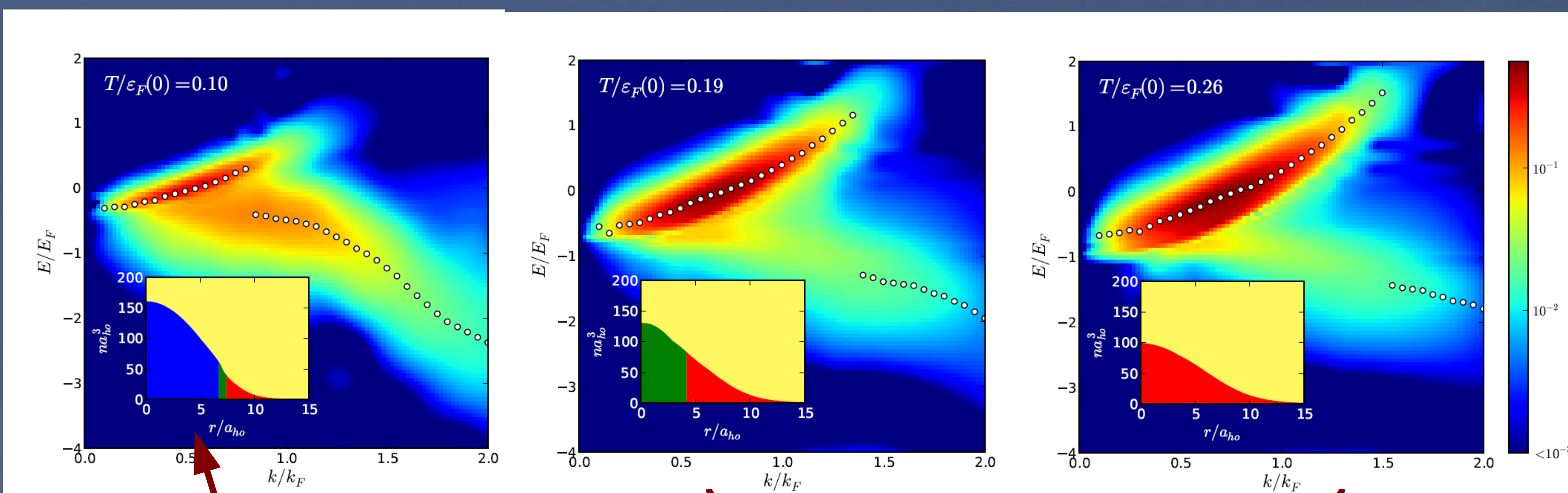
$$\mathrm{EDC}(p,E,T) = \mathcal{C}p^2 \int_0^\infty dr\, r^2 \frac{1}{\varepsilon_F(r)} A\left[\frac{p}{p_F(r)}, \frac{E-\mu(r)}{\varepsilon_F(r)}, \frac{T}{\varepsilon_F(r)}\right] f(E-\mu(r)),$$

Energy Distribution Curve (accessible experimentally)

Normalization factor

Local Density Approximation

Only occupied branch accessible



Density profile for JILA trap (blue-SF, green-PG, red-NOR)

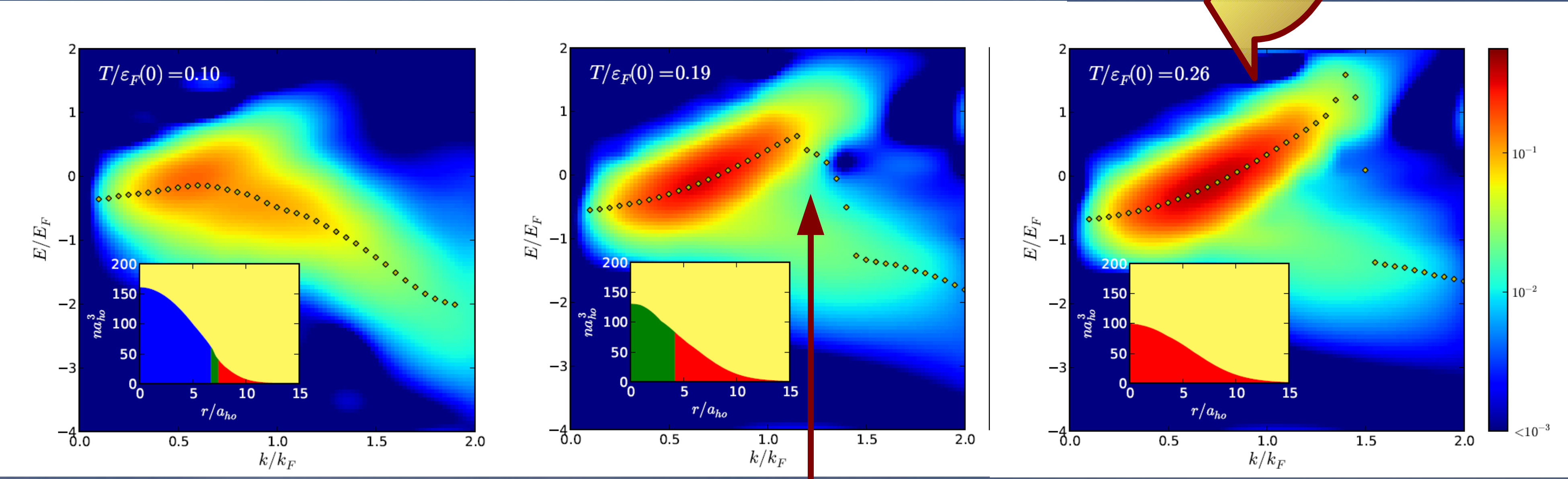
No “back-bending”

Expected EDC signal for $1/ak_F$=0.2 (BEC side)

Momentum-resolved rf spectroscopy

does not change. The length of the rf pulse limits our energy resolution to approximately $0.2E_F$. As described

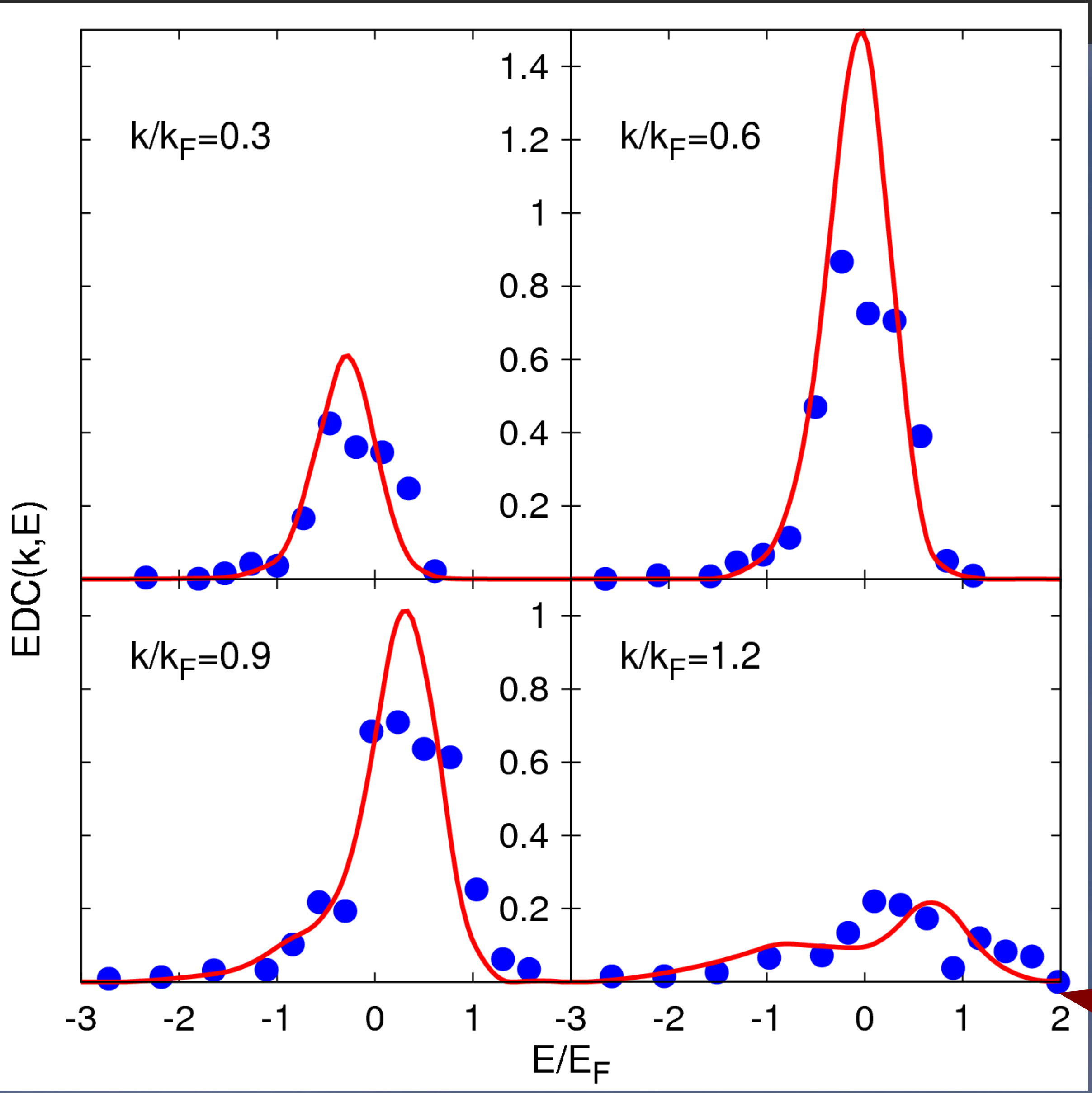
gap regime. In the intensity plots, white dots indicate the centers derived from unweighted gaussian fits to each of the energy distribution curves, or EDCs, (vertical trace at a given wave vector). The energy dispersion mapped



"back-bending" structure

Expected EDC signal for $1/ak_F$=0.2 (BEC side)

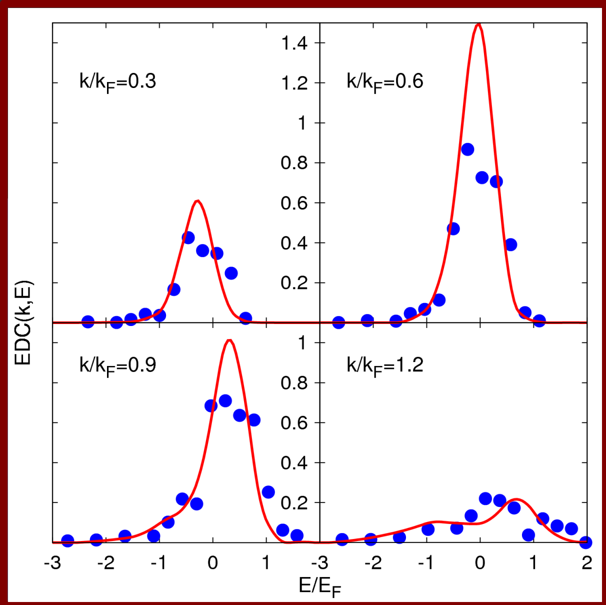
QMC vs Experiment



Experimental* (dots) and theoretical (lines) energy distribution curves (EDC) for the trapped atomic gas in the **unitary regime at the critical temperature** (defined in the center of the trap) for various wave vectors k.

Theoretical results do not contain any fitted parameters which could be used to adjust to experiment!

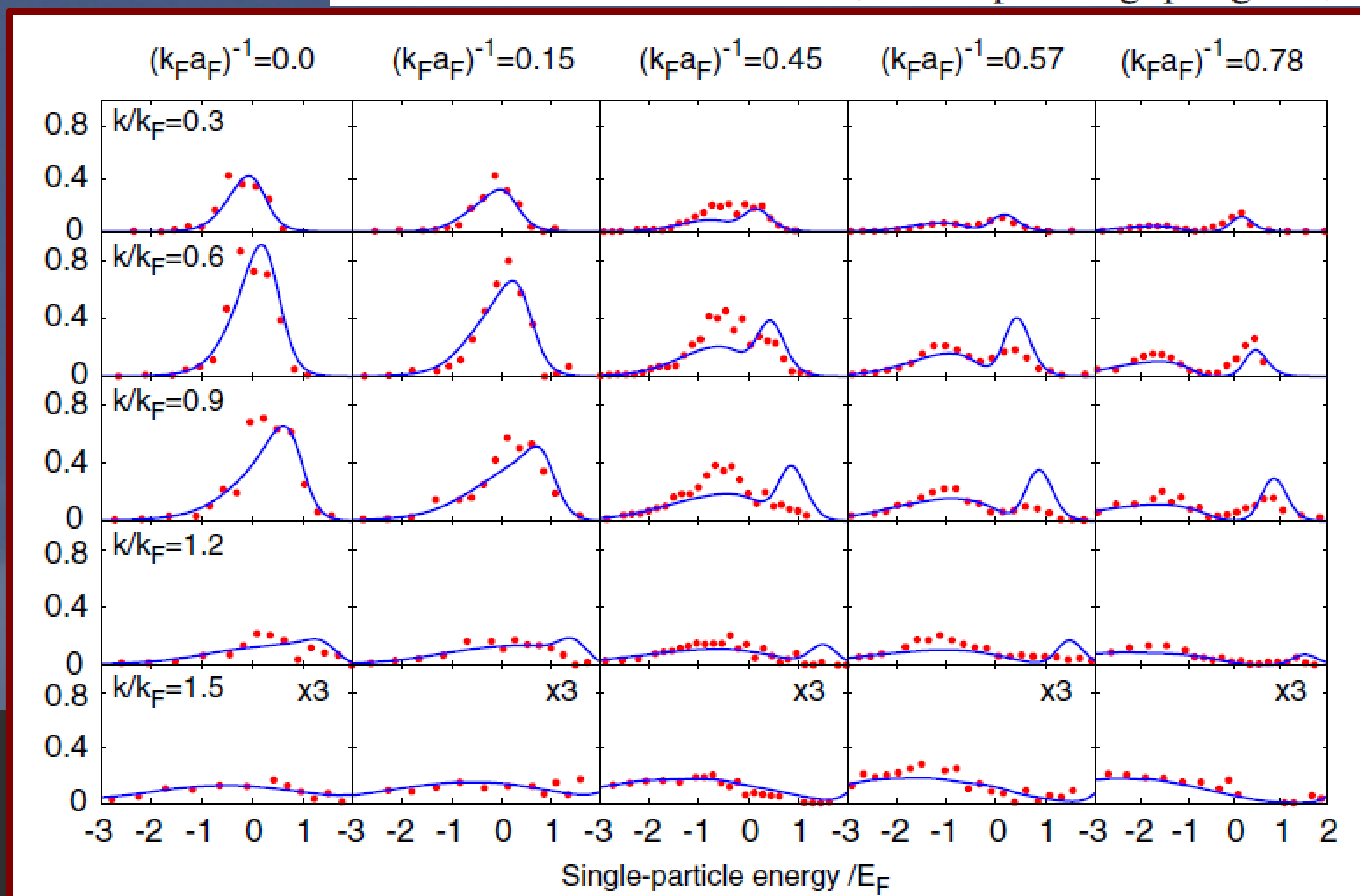
* J. P. Gaebler, *et al.*, Nature Physics 6, 569 (2010);
A. Perali, *et al.*, Phys. Rev. Lett. 106, 060402 (2011)

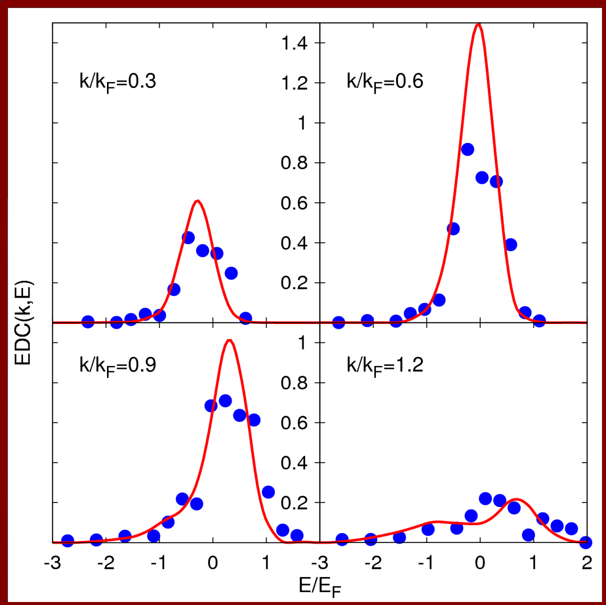


Theory vs Experiment

Perali, A., Palestini, F., Pieri, P., Strinati, G.C., Stewart, J.T., Gaebler, J.P., Drake, T.E. & Jin, Phys. Rev. Lett. 106, 060402 (2011)

In this work, we present a theoretical investigation of the pseudogap regime based on the *t*-matrix pairing-fluctuation approach of Ref. [3], addressing both the single-particle spectral function and the thermodynamics of the gas, as a function of interaction strength in the BCS-BEC crossover. We find that, in the pseudogap regime, the





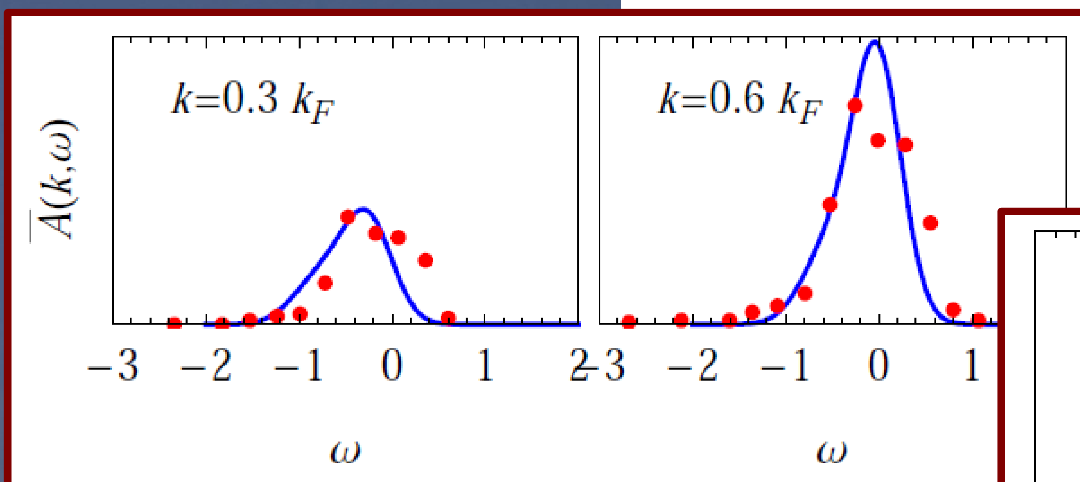
Theory vs Experiment

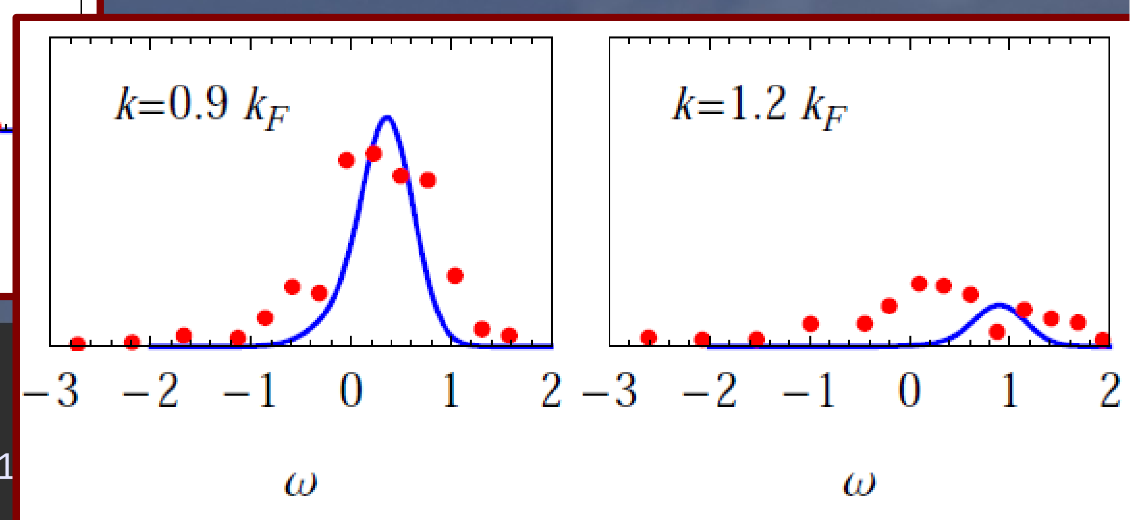
Nascimbene, S., Navon, N., Pilati, S., Chevy, F., Giorgini, S., Georges, A. & Salomon, C., arXiv:1012.4664v1

In the vicinity of the Fermi surface, the dispersion relation of the Fermi liquid quasi-particles reads

$$\hbar\omega_k = \mu + \frac{\hbar^2 k^2 - \hbar^2 k_F^2}{2m^*}, \qquad (3)$$

where $m^* = 1.13\, m$. Assuming long-lived quasiparticles, we approximate $A(k,\omega)$ by $\delta(\omega - \omega_k)$ and perform the





Conclusions

- **The pairing gap** and quasiparticle spectrum was determined in ***ab initio* calculations** at zero and finite temperatures.
- The system **is NOT a BCS superfluid (**similarity with high-Tc superconductors).
- **Unitary Fermi gas** demonstrates the **pseudogap** behavior.
- **Agreement** between **experimental and theoretical data** has been found.