The Abdus Salam International Centre for Theoretical Physics

United Nations Educational, Scientific and Cultural Organization

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2030-1

Conference on Research Frontiers in Ultra-Cold Atoms

4 - 8 May 2009

Theory of radio-frequency spectroscopy of ultracold Fermi atoms

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"Research Frontiers in Ultra-Cold Atoms"
ICTP, Trieste, May 4-9, 2009

References:

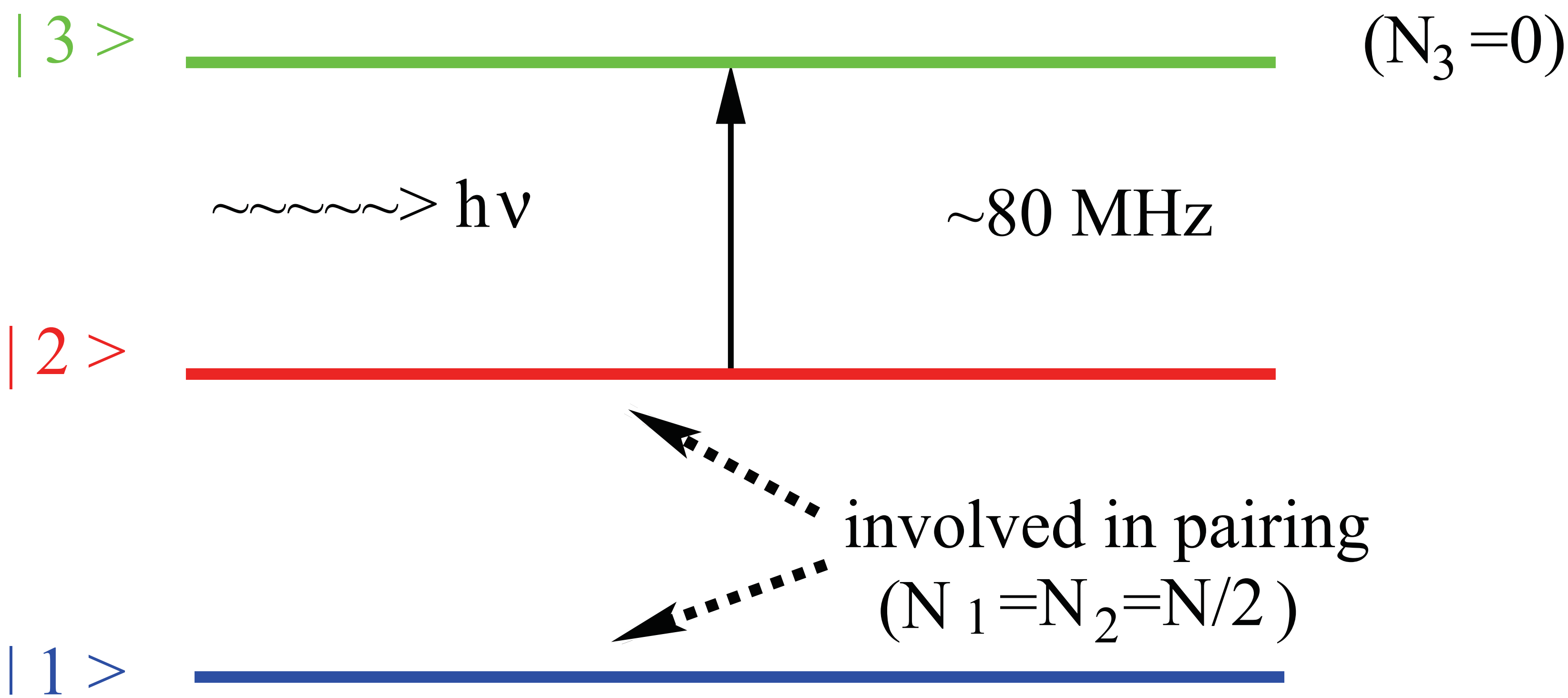
[1] A. Perali, P. Pieri, and G.C. Strinati,
Phys. Rev. Lett. **100**, 010402 (2008):
"Competition between final state and pairing gap effects in the radio-frequency spectra of ultracold Fermi atoms" [below T_c]

[2] P. Pieri, A. Perali, and G.C. Strinati,
preprint at http://arxiv.org/abs/0811.0770:
"Enhanced paraconductivity-like fluctuations in the radio frequency spectra of ultracold Fermi atoms" [above T_c]

Original motivation (from experiments):

Jin (2003), Grimm (2004), Ketterle (2003-2008)

Atomic (^{6}Li,^{40}Na) energy levels in a magnetic field:



Questions:

1) From the shape of RF spectra, is it possible to extract the value of the "pairing gap" (order parameter below T_c, pseudo-gap above T_c, $\cdots$) ?

No interaction: $h\nu = \varepsilon_3 - \varepsilon_2$

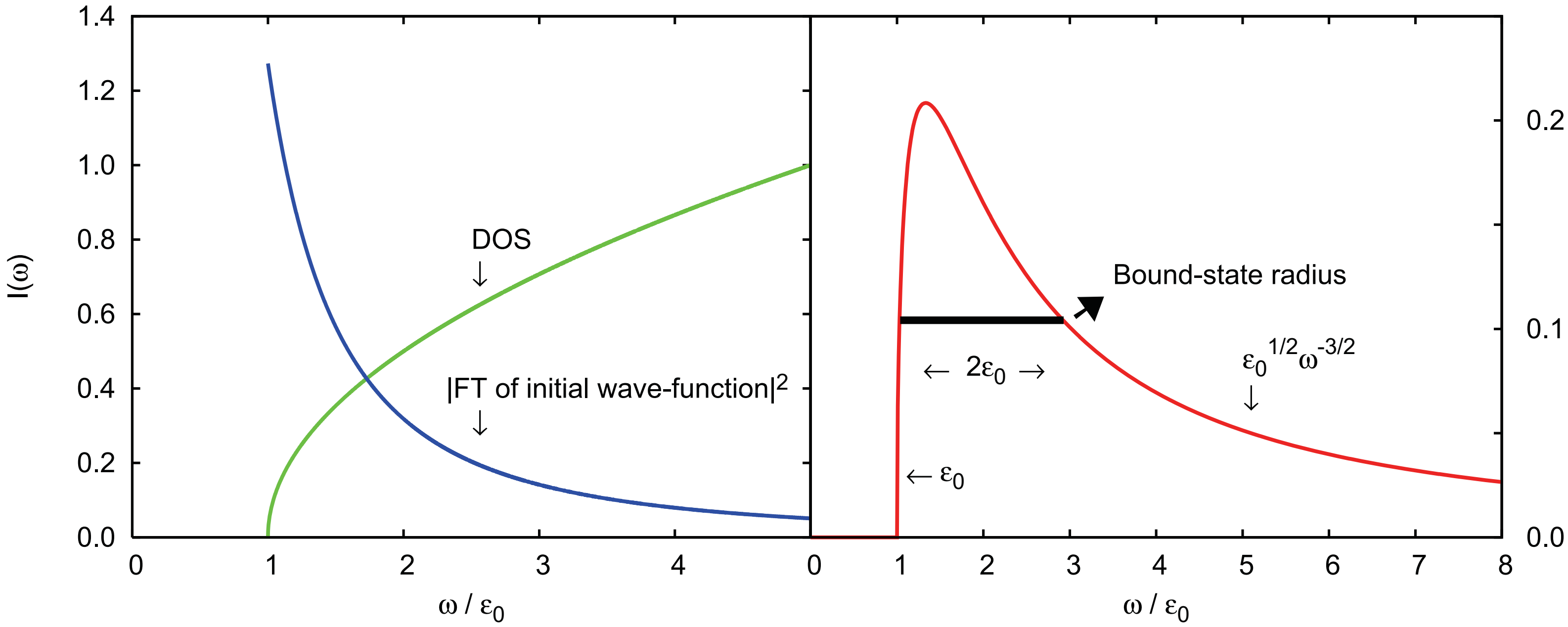
$|1>$ and $|2>$ interact: $h\nu \neq \varepsilon_3 - \varepsilon_2$ (pairing)

$|1>$ and $|3>$ interact: (final-state effects)

2) To what extent final-state effects affect the RF spectra ?

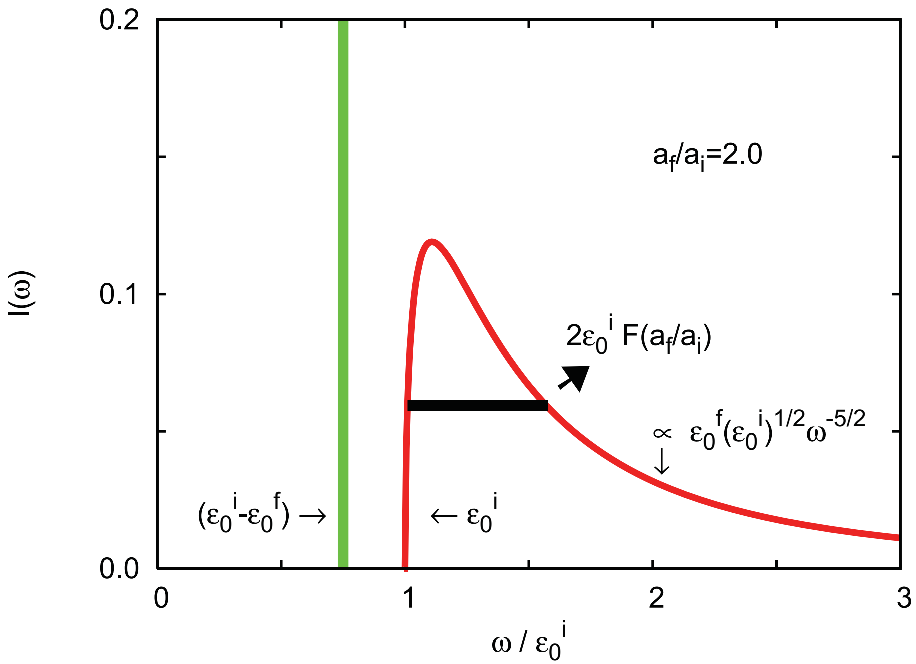
Learning from the molecular calculation (Chin & Julienne - 2005):

When $a_f = 0 \implies$ RF spectrum $\propto$ density of final states $\times$ |FT of initial wave function|^2



$\implies$ extract binding energy from threshold & bound-state radius from width of half-maximum

When $a_f \neq 0 \implies$ RF spectrum:



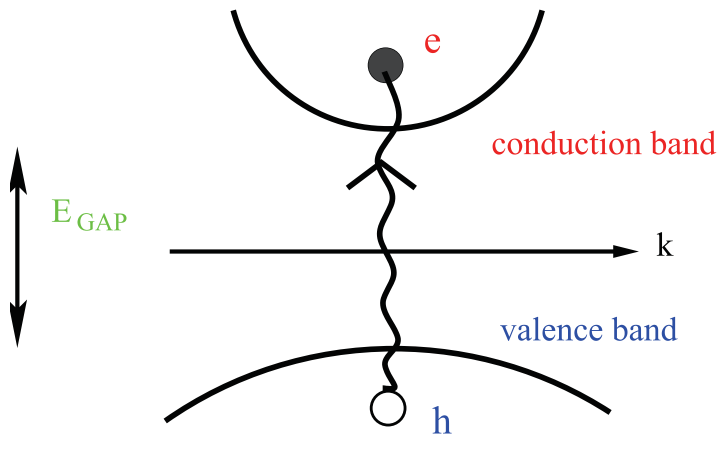
Piles up at threshold

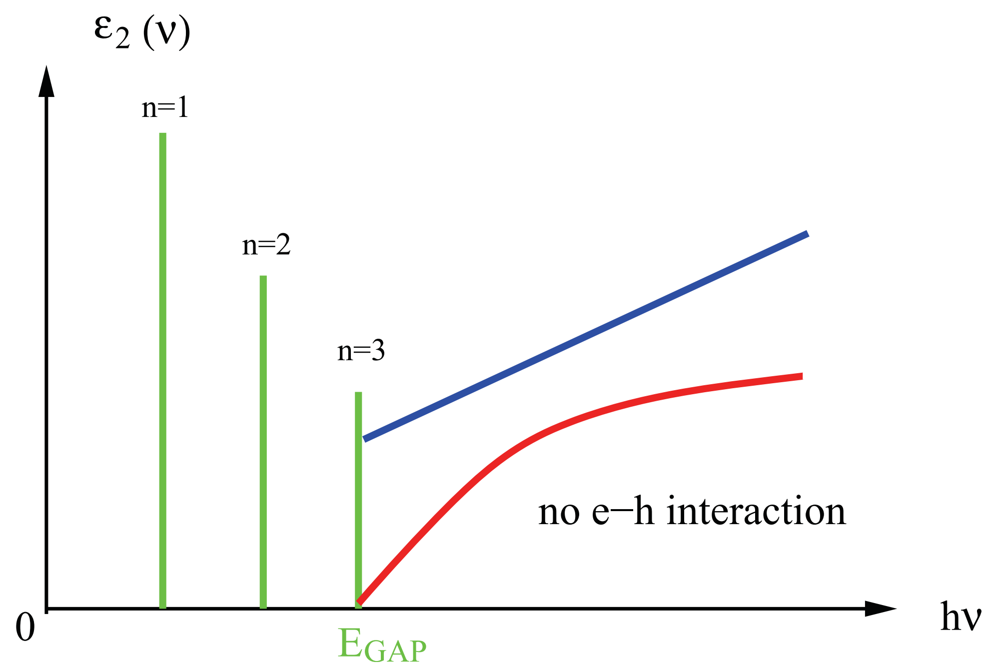
Tail decays faster

Bound peak (.|.) appears

Total area is preserved

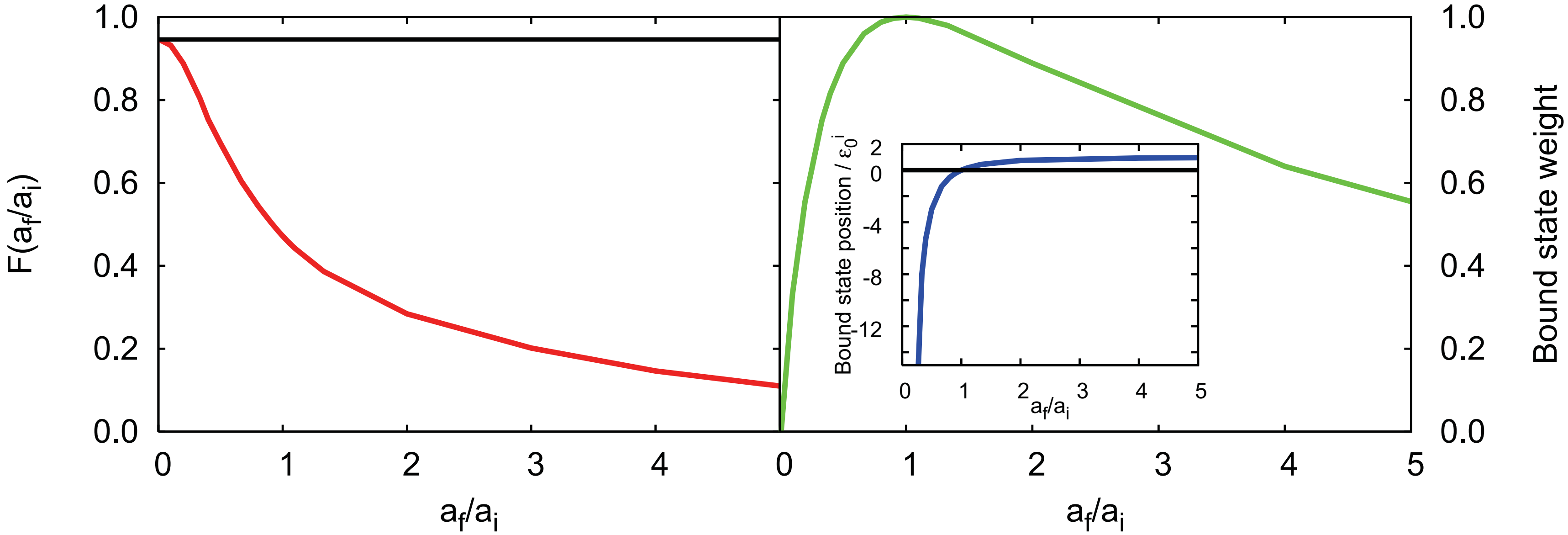
Analogy with Excitonic Effect in Semiconductors:





$\Longrightarrow$ competition between finite-gap ($\longrightarrow$) and excitonic ($\longleftarrow$) effects !

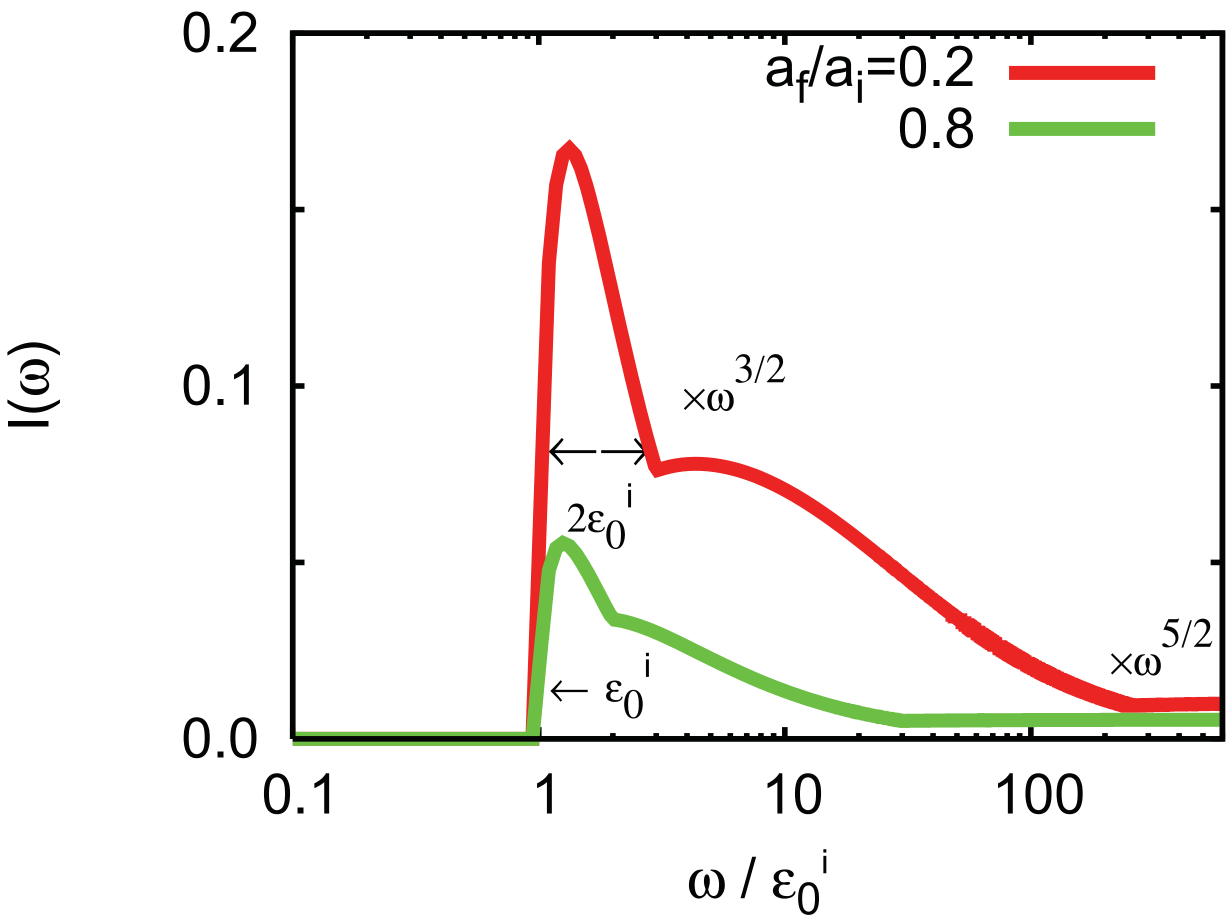
Characteristics of molecular spectra:



$\Longrightarrow$ suggestion : when a_f is sufficiently $\neq a_i$

- The position of the bound peak recedes away from threshold

- A frequency window opens up in the continuum, where the spectrum "resembles" the one with $a_f = 0$!



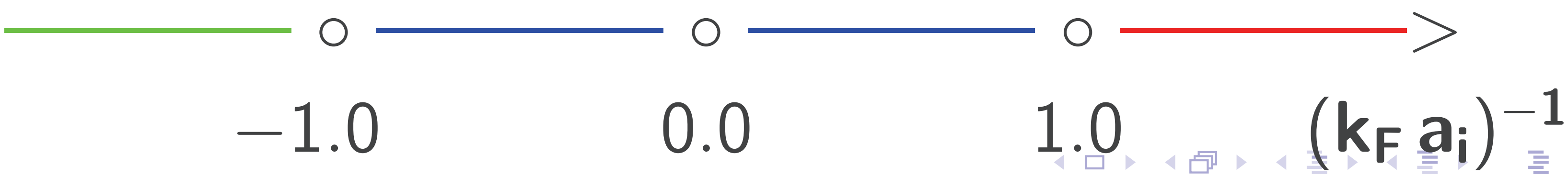
Single molecule ⇒ many-body system:

Question: How does one extend the molecular calculation to finite density n and temperature T ?

In this case, by varying a_i across a Fano-Feshbach resonance, one realizes the BCS-BEC crossover:

$a_i < 0,\ k_F\lvert a_i\rvert \lesssim 1$	$0 < a_i,\ k_F a_i \lesssim 1$
BCS limit of Cooper pairs	BEC limit of composite bosons

(k_F = Fermi wave vector related to n)



Recovering the molecular RF spectra from the many-body RF spectra:

In BEC limit, the many-body RF spectrum $I_N(\omega)$ is related to molecular RF spectrum $I_0(\omega)$ as follows:

$$I_N(\omega) = N_{\rm mol}\, I_0(\omega) \quad (N_{\rm mol} = \text{number of molecules})$$

For the many-body system, $N_{\rm mol}$ is obtained as:

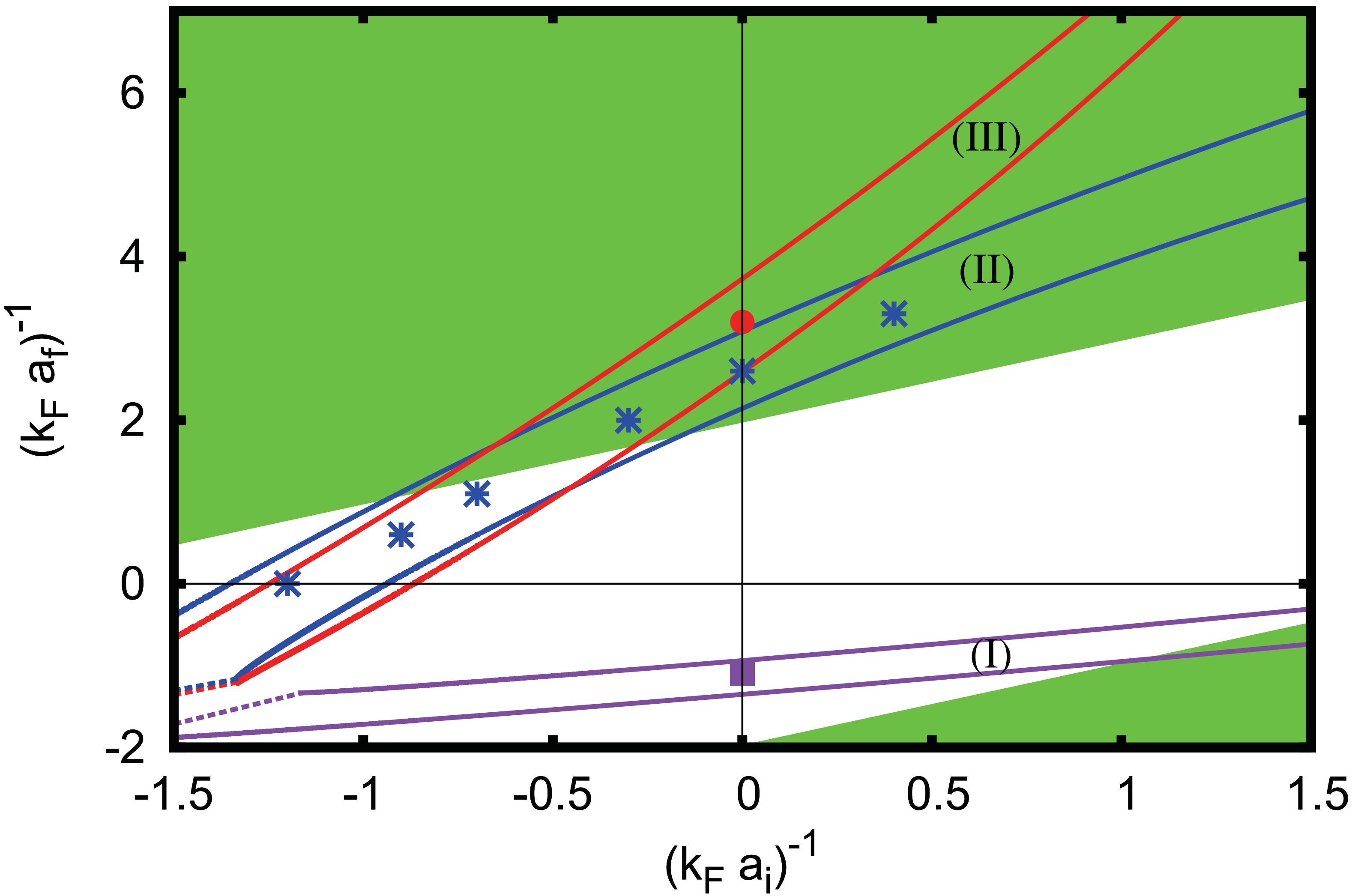
$$N_{\rm mol} \approx N_0 \quad (\text{condensate}) \;\; \textit{for } T \ll T_c$$
$$N_{\rm mol} \approx N' \quad (\text{non} - \text{condensate}) \;\; \textit{for } T \approx T_c$$

$\Rightarrow$ different "many-body diagrams" are expected to be important in the two temperature regimes !

Use this as a criterion to “classify” the theory work on many-body RF spectra:

Group (year)	a_i	a_f	N_0	N'
Törma (2004)	yes	no	yes	no
Griffin (2005)	yes	no	yes	no
Levin (2005)	yes	no	yes	no
Bruun & Stoof (2008)	yes	no	yes	no
Yu & Baym (2006)	yes	yes	yes	no
Strinati (2008)	yes	yes	yes	no
Mueller (2008)	yes	yes	yes	no
Levin (2009)	yes	yes	yes	no
Strinati (2009)	yes	yes	no	yes

Experimental coupling plane for $^6\mathrm{Li}$:



The system Hamiltonian (^{6}Li):

Deal with "broad" Fano-Feshbach resonances.

- Bare contact interaction v_{12} between spins "1" and "2" $\Rightarrow$ regularize it via the scattering length $a_{12} \leftrightarrow a_i$ (initial-state effects)
- Bare contact interaction v_{13} between spins "1" and "3" $\Rightarrow$ regularize it via the scattering length $a_{13} \leftrightarrow a_f$ (final-state effects)
- Bohr frequency $\omega_{32} = \varepsilon_3 - \varepsilon_2$ between "bare" atomic levels 3 and 2
- Two chemical potentials:
  $\mu \leftrightarrow$ common to spins "1" and "2" $(N_1 = N_2)$
  $\mu_3 \leftrightarrow$ spin "3" $(N_3 = 0)$

What does an RF experiment measure?

$\frac{dN_3(t)}{dt}$ as induced by the perturbing Hamiltonian:

$$H'(t) = \gamma \int d\mathbf{r}\, e^{i(\mathbf{q}_{RF}\cdot\mathbf{r} - \omega_{RF} t)}\, \psi_3^\dagger(\mathbf{r})\psi_2(\mathbf{r}) + h.c.$$

$\mathbf{q}_{RF} \approx 0$ and ω_{RF} = frequency of RF radiation.

$\frac{dN_3(t)}{dt}$ is related to the current operator:

$$\begin{aligned} I(t) &= i[H'(t), N_3] \\ &= -i\gamma \int d\mathbf{r}\, e^{i(\mathbf{q}_{RF}\cdot\mathbf{r} - \omega_{RF} t)}\, \psi_3^\dagger(\mathbf{r})\psi_2(\mathbf{r}) + h.c. \end{aligned}$$

Within linear-response theory ...

... one ends up with the (retarded $\leftrightarrow R$) spin-flip correlation function:

$$\Pi^R(\mathbf{r},\mathbf{r}';t-t') = -i\theta(t-t')\langle[B(\mathbf{r},t),B^\dagger(\mathbf{r}',t')]\rangle$$

where $B(\mathbf{r},t) = e^{iKt}\psi_2^\dagger(\mathbf{r})\psi_3(\mathbf{r})e^{-iKt}$ $\Longrightarrow$

the RF spectrum is given by

$$I(\omega_{th}) = -2\gamma^2 \int d\mathbf{r}\, d\mathbf{r}'\, \mathrm{Im}\{\Pi^R(\mathbf{r},\mathbf{r}';\omega_{th})\}$$

where $\omega_{th} = \omega_{RF} + \mu - \mu_3$ is a "theoretical" detuning frequency.

Connection with the diagrammatic PT:

As usual, one needs to introduce the Matsubara counterpart of the retarded correlation function:

$$\Pi(\mathbf{r}, \mathbf{r}'; \omega_\nu) = \int_0^\beta d\tau \, e^{i\omega_\nu \tau}$$

$$\times \quad \langle T_\tau \left[\psi_2(\mathbf{r}', 0) \psi_2^\dagger(\mathbf{r}', \tau^+) \psi_3(\mathbf{r}, \tau) \psi_3^\dagger(\mathbf{r}', 0^+) \right] \rangle$$

where $\omega_\nu = 2\pi\nu/\beta$ [ν integer and $\beta = (k_B T)^{-1}$]
and T_τ = imaginary time-ordering operator $\Longrightarrow$

analytic continuation in the complex $\omega_{th}-$plane.

A quite difficult part of the whole story !
($\leftrightarrow$ sometimes recourse to Padé approximants)

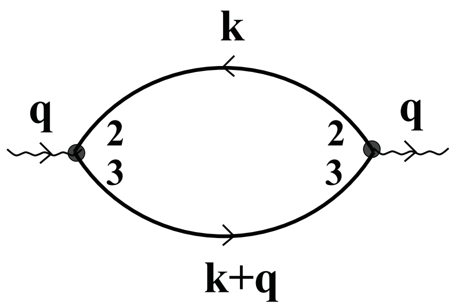
Hierarchy of approximations below T_c:

- $\boxed{a_i = 0\,,\, a_f = 0}$ $\Longrightarrow$ non-interacting atoms
  RF spectrum is a delta spike at $\omega_{RF} = \omega_{32}$
  take this as the "reference frequency" $\Longrightarrow$
  $\omega_{\text{exp}} = \omega_{RF} - \omega_{32}$

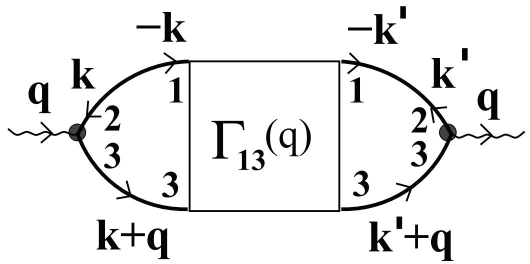
- $\boxed{a_i \neq 0\,,\, a_f = 0}$ $\Longrightarrow$ atom in initial state "2" correlates with its mate in "1" within the BCS approximation $\Longrightarrow$ RF spectrum is obtained from the BCS bubble

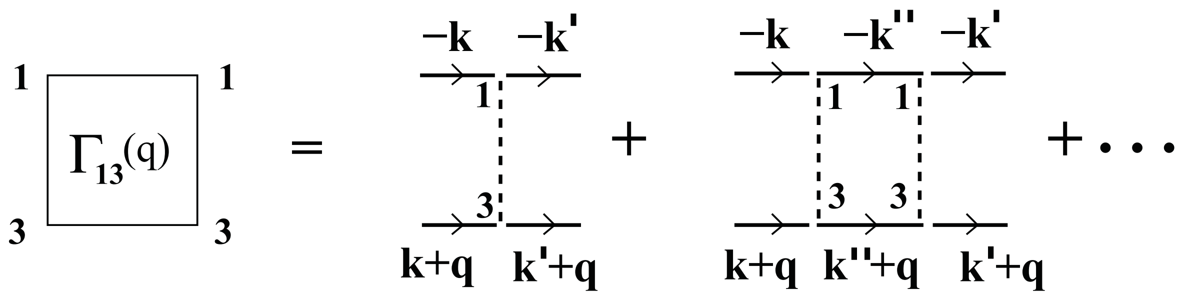
BCS & BCS-RPA diagrams below T_c:

(a)

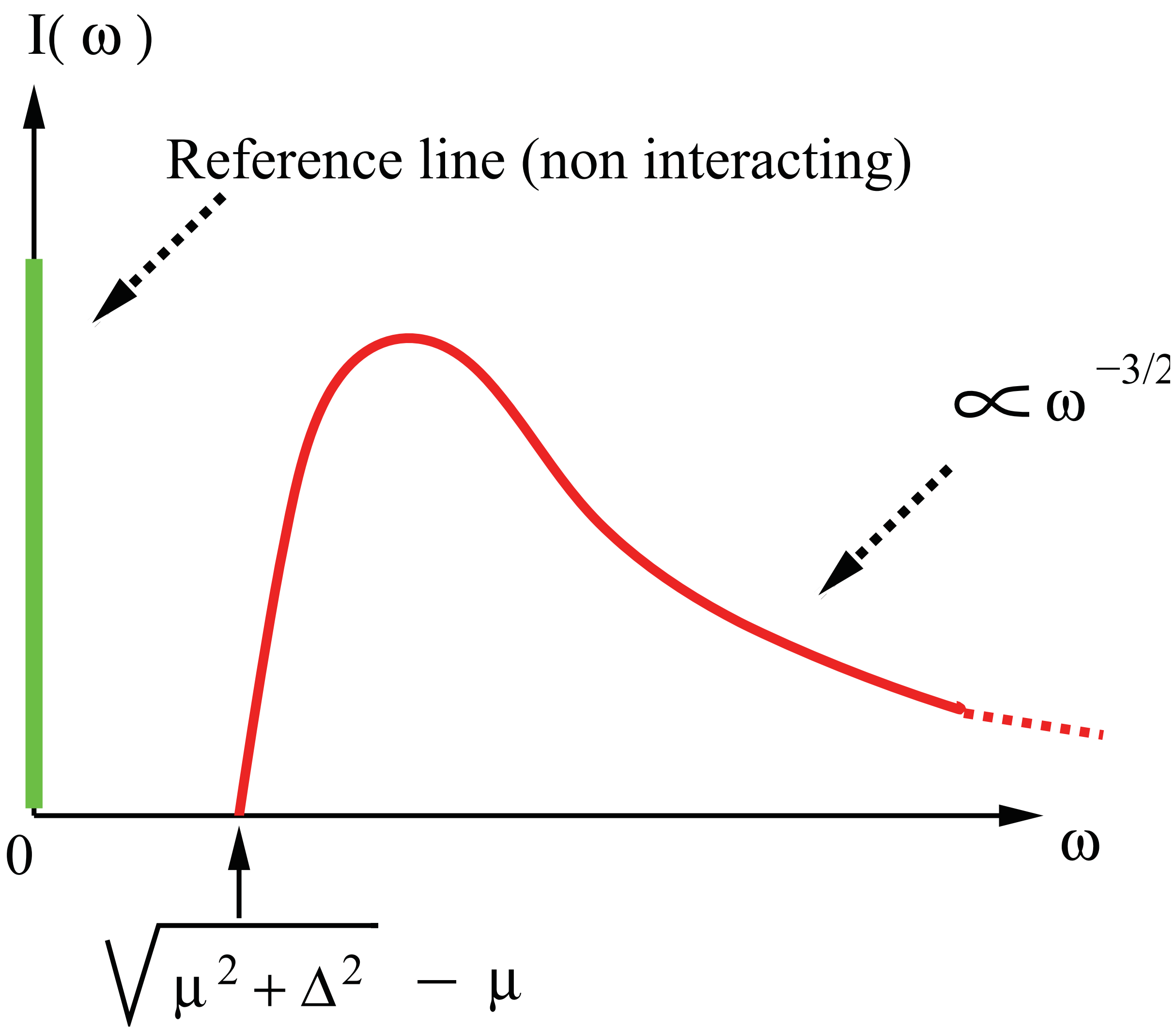


(b)





RF spectrum from BCS bubble at $T = 0$:



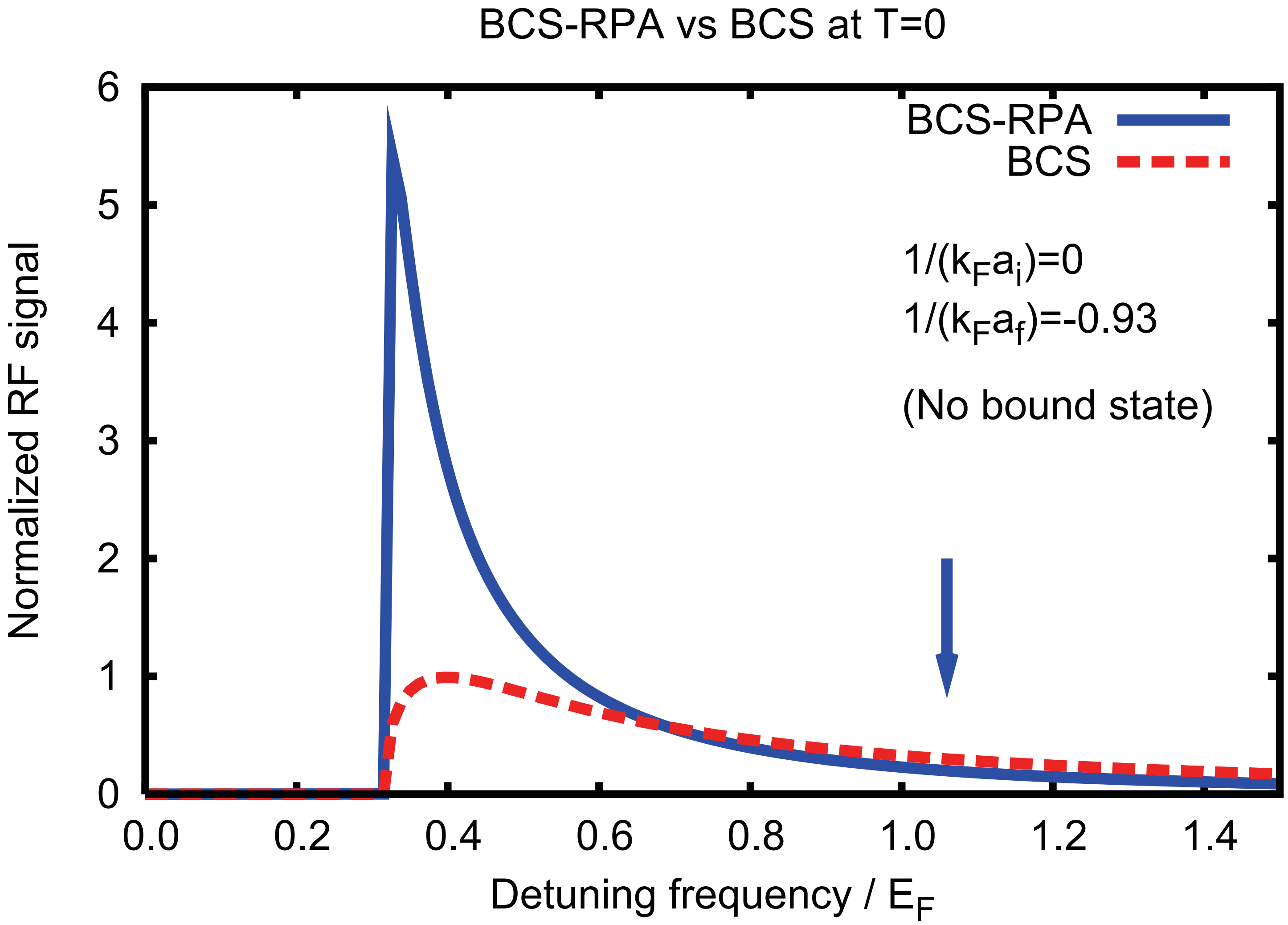
Hierarchy of approximations below T_c: (II)

- $\boxed{a_i \neq 0\,,\, a_f \neq 0}$ $\implies$ in addition, atom in final state "3" interacts with atom left behind in state "1" $\implies$ the RF spectrum is obtained from the BCS-RPA series

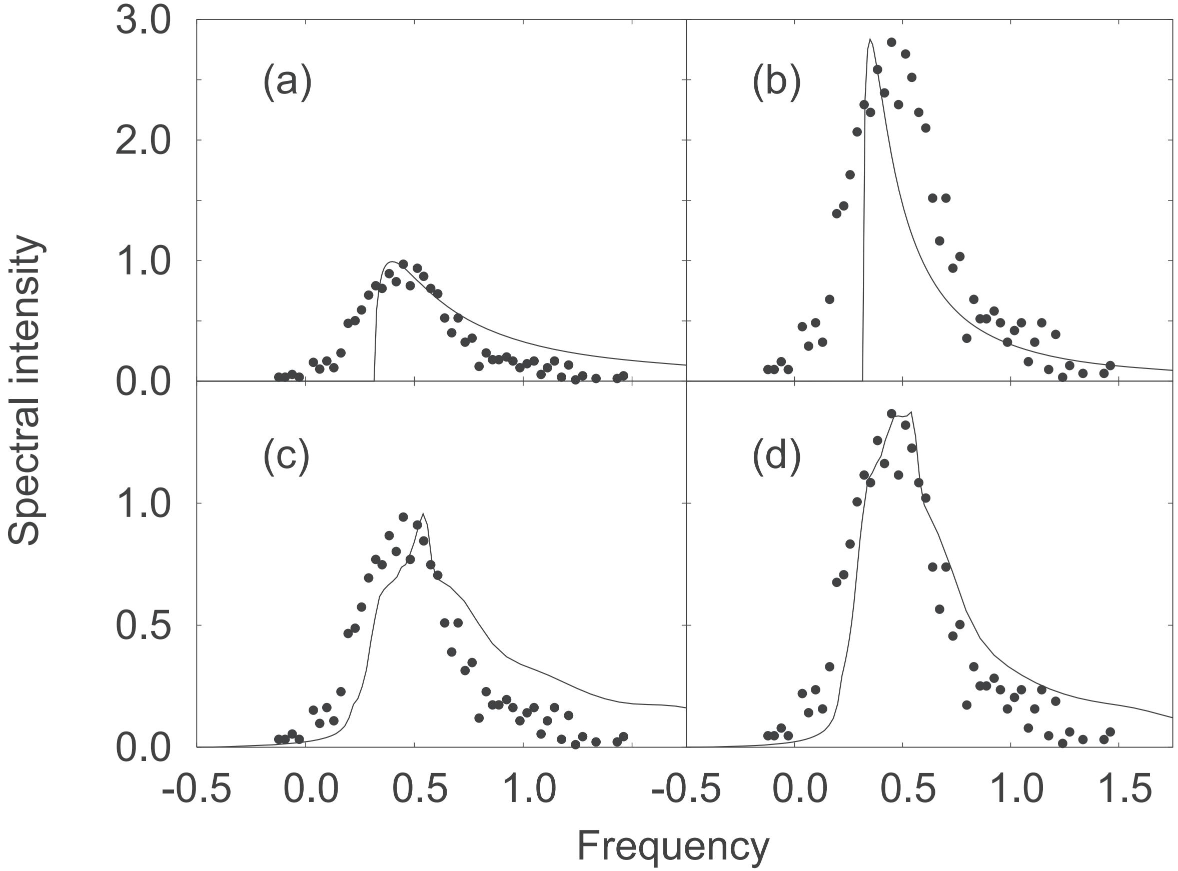
- In both cases (BCS & BCS-RPA), in the BEC limit we get:

$$N_{\mathrm{mol}} \leftrightarrow N_0 = \mathrm{Volume} \times \left(\frac{m^2 a_i}{8\pi}\right) \Delta^2_{BCS}$$

RF spectrum from BCS-RPA at $T = 0$:



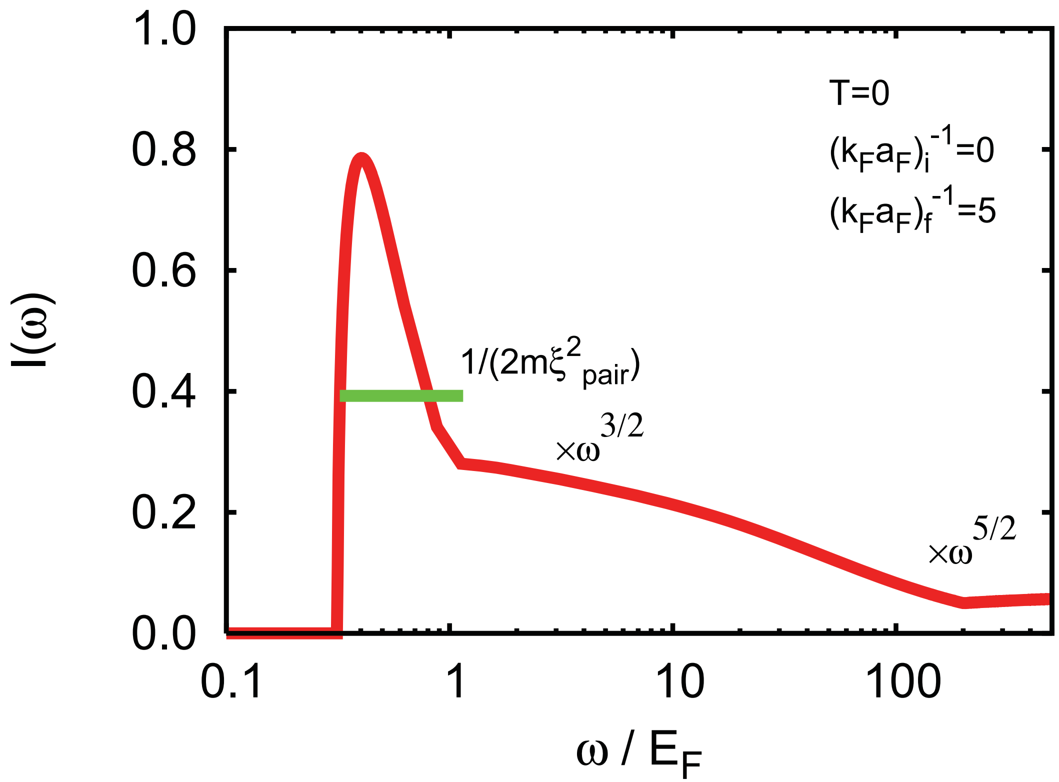
Comparison with experiments below T_c:



$$(k_F a_i)^{-1} = 0 \qquad (k_F a_f)^{-1} = -1.32 \qquad T \lesssim 0.5\, T_c$$

[Exp. data: Fig.2(d) of PRL **99**, 090403 (2007)]

When a_f is quite different from a_i:



- "Pair size" from width of half-maximum [Ketterle & al., Nature **454**, 739 (2008)]
- Energy scale Δ_{BCS} (or Δ_∞ - see below) from "intermediate-frequency plateau"

Hierarchy of approximations above T_c:

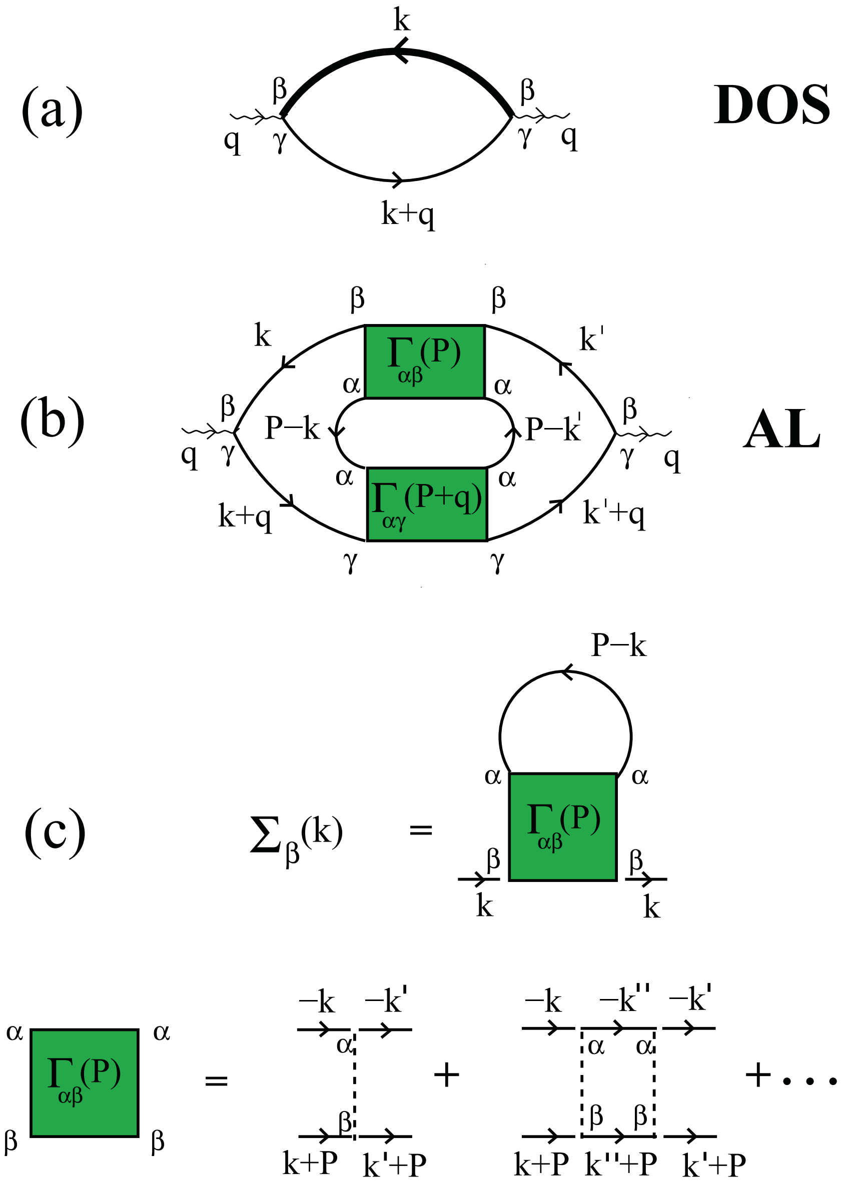
The self-energy $\Sigma(k)$ with "pairing fluctuations" plays a crucial role $\Longrightarrow$ for atoms "2" interacting with atoms "1"

$$\boxed{\Sigma_2(k) = -\int dq\, \Gamma_{21}(q)\, \mathcal{G}_1(q-k)}$$

- $\boxed{a_i \neq 0\,,\, a_f = 0}$ $\Longrightarrow$ RF spectrum is obtained

  from the DOS (density-of-states) diagram

DOS & AL diagrams above T_c:



Hierarchy of approximations above T_c: (II)

- $\boxed{a_i \neq 0\,,\, a_f \neq 0} \implies$ RF spectrum is obtained from the AL (Aslamazov-Larkin) diagram with two different pairing propagators:

$$\Gamma_{21}\ (\leftrightarrow a_i) \quad \text{and} \quad \Gamma_{31}\ (\leftrightarrow a_f)$$

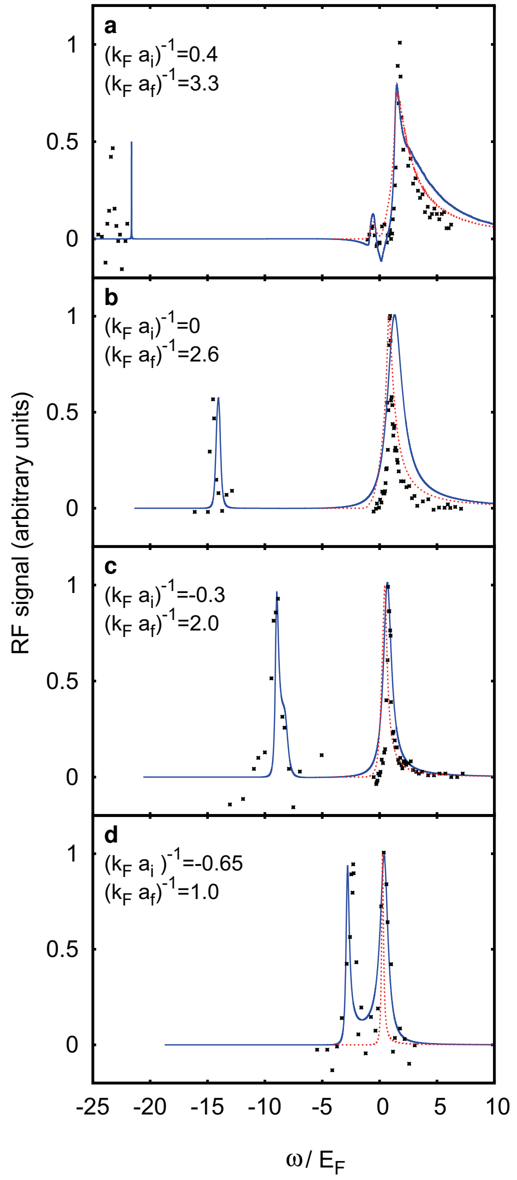
- AL diagram requires use of Padé approximants !
- In both cases (DOS & AL), in the BEC limit:

$$N_{\rm mol} \leftrightarrow N' = \text{Volume} \times \left(\frac{m^2\, a_i}{8\pi}\right) \Delta_\infty^2$$

with $\Delta_\infty^2 = \int dq\, e^{i\omega_\nu \eta}\, \Gamma_{21}(q)$

- Definition of Δ_∞ holds for arbitrary couplings.

Comparison with experiments for $T \approx T_c$:



$$\frac{1}{k_F a_i} = 0.4 \quad \frac{1}{k_F a_f} = 3.3 \quad (*)$$

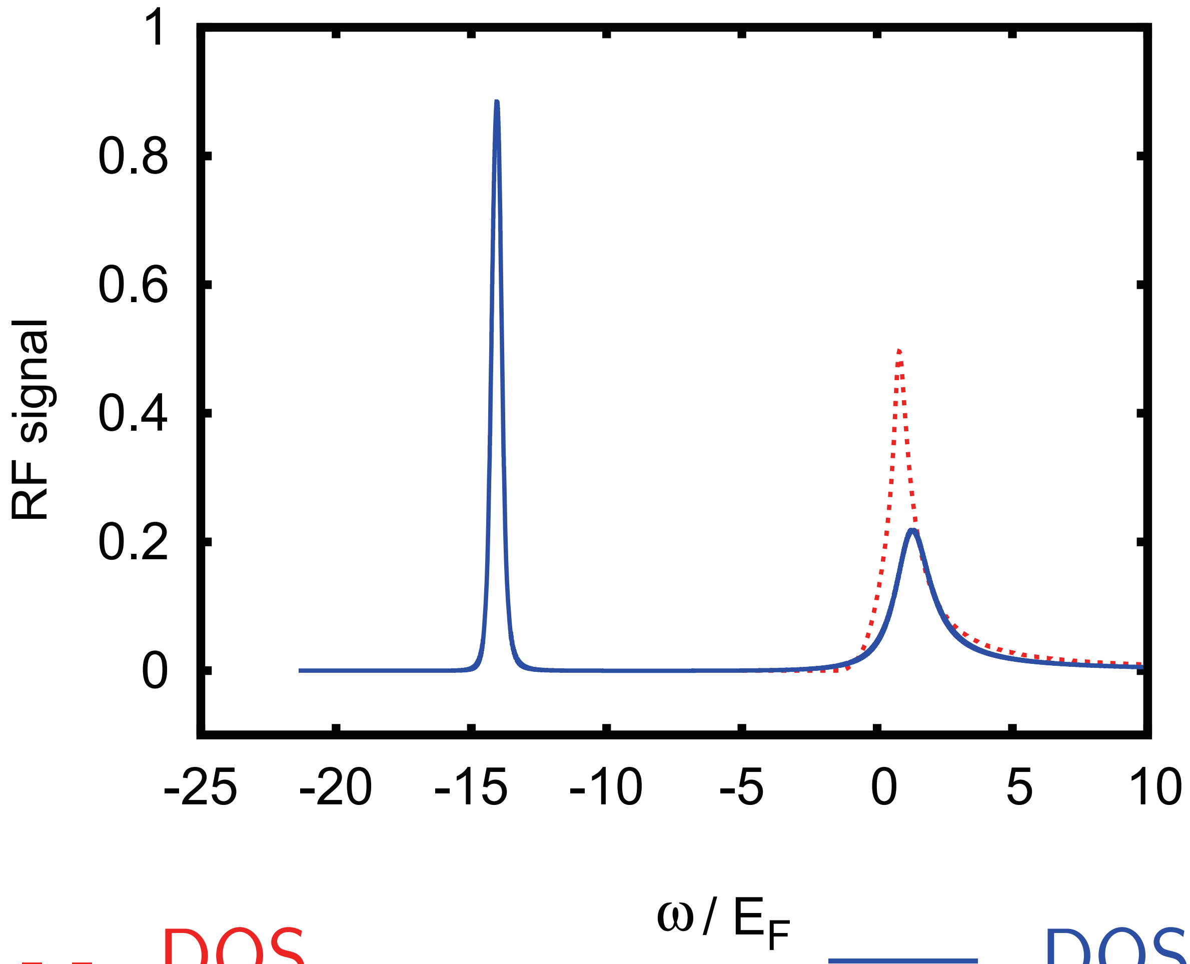
$$\frac{1}{k_F a_i} = 0.0 \quad \frac{1}{k_F a_f} = 2.6 \quad (*)$$

$$\frac{1}{k_F a_i} = -0.3 \quad \frac{1}{k_F a_f} = 2.0 \quad (*)$$

$$\frac{1}{k_F a_i} = -0.65 \quad \frac{1}{k_F a_f} = 1.0 \quad (*)$$

[Exp. data from Fig.4 of Nature **454**, 739 (2008)]

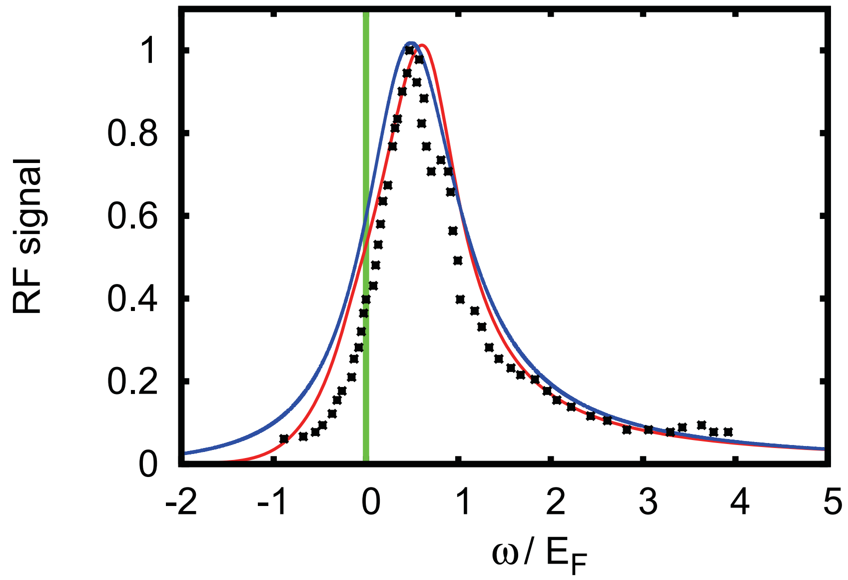
Comparison between DOS and DOS+AL on an absolute scale:

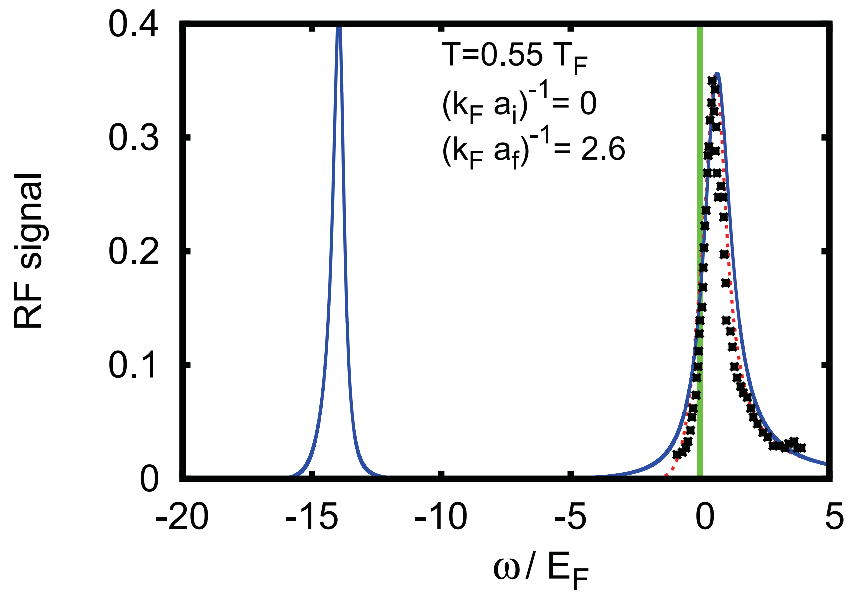


- - - DOS —— DOS + AL

$\frac{1}{k_F a_i} = 0.0$ $\frac{1}{k_F a_f} = 2.6$ $T \approx T_c$

Further comparison with data ($T \approx T^*$):

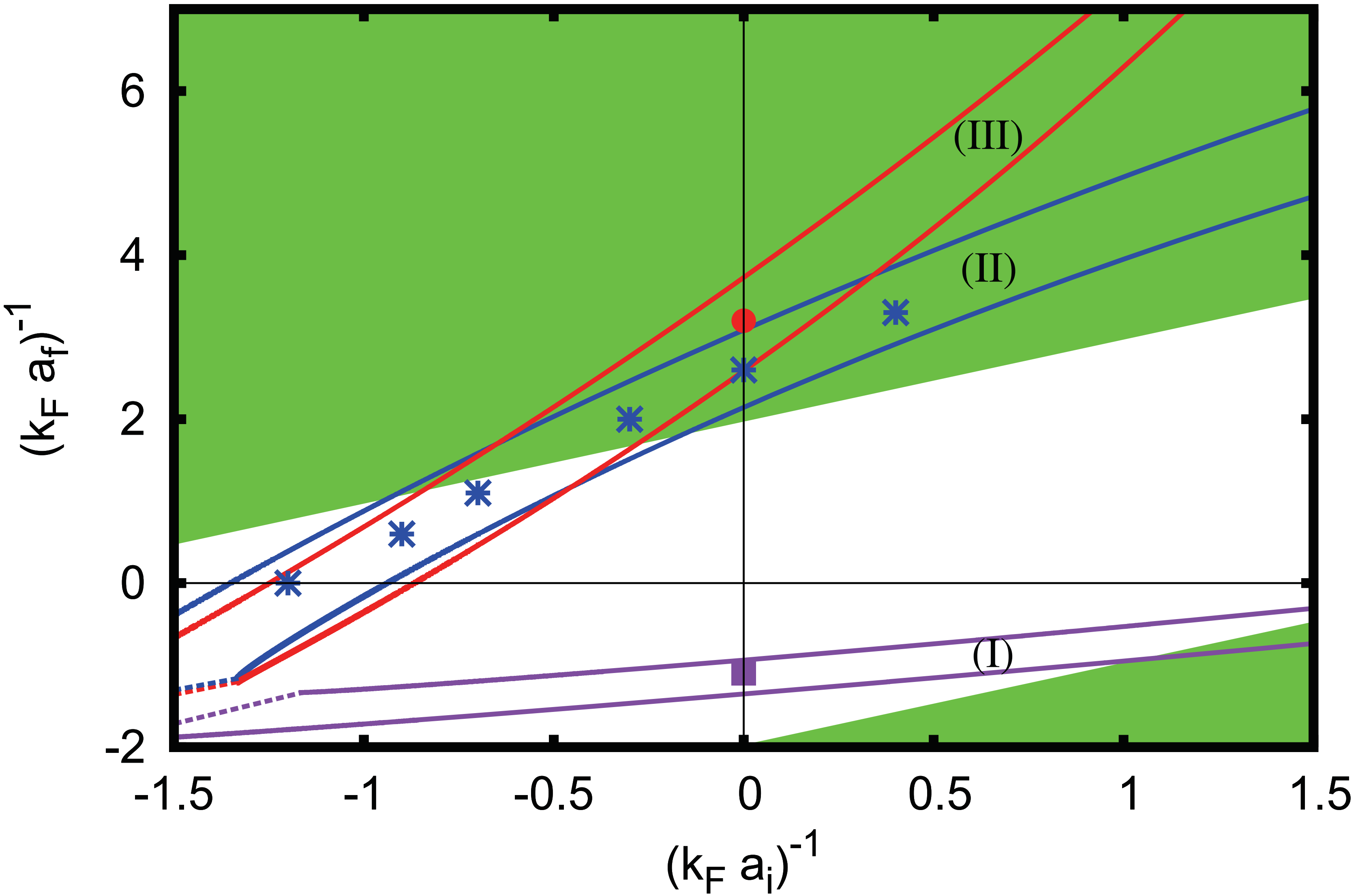




[Exp. data from Fig.8(d) of arXiv:0808.0026v2 - Ketterle]

$\Longrightarrow$ do not forget about the presence of the bound state with DOS+AL !

We are here (∗) ↙ :



What do we learn from the RF spectra?

Information about the pair-correlation function:

$$g_{\uparrow\downarrow}(\mathbf{r}) = \langle \psi^\dagger_\uparrow(\mathbf{r})\psi^\dagger_\downarrow(0)\psi_\downarrow(0)\psi_\uparrow(\mathbf{r})\rangle - \left(\frac{n}{2}\right)^2$$

- Small-**r** behavior:

$$\lim_{\mathbf{r}\to 0} \mathbf{r}^2 g_{\uparrow\downarrow}(\mathbf{r}) = \left(\frac{m\Delta}{4\pi}\right)^2$$

where $\Delta \longleftrightarrow$ BCS gap Δ_{BCS} , or Δ_∞ , or a combination of both.

- Average spatial behavior in terms of

$$\xi^2_{\text{pair}} = \frac{\int d\mathbf{r}\,\mathbf{r}^2\, g_{\uparrow\downarrow}(\mathbf{r})}{\int d\mathbf{r}\, g_{\uparrow\downarrow}(\mathbf{r})}$$

Conclusions:

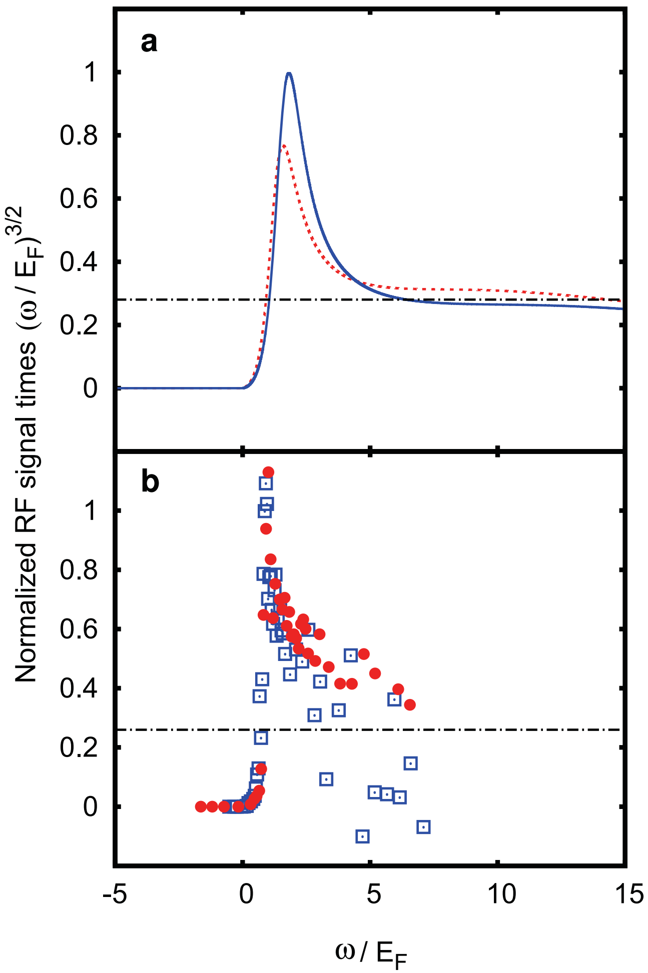
- ♣ Inclusion of final-state effects is essential for a correct understanding of the RF spectra of ultra-cold Fermi atoms.
- ♣ There exists a competition between pairing-gap ($\longrightarrow$) and excitonic ($\longleftarrow$) effects.
- ♣ BCS bubble $\bigoplus$ BCS-RPA diagrams at low T.
- ♣ DOS with pairing self-energy $\bigoplus$ AL diagrams above T_c (possibly needed also below T_c).
- ♣ Extract from RF spectra information about the pair-correlation function.

Additional material: Extracting Δ_∞ from "tail" of RF spectra

In the green region of the coupling plane , it is possible to extract the quantity Δ_∞ from the RF spectra via the following "prescription" :

- Normalize the continuum peak to its own area
- Multiply the resulting spectrum by $\left(\frac{\omega}{E_F}\right)^{3/2}$
- From the intermediate plateau read off the value $\frac{3}{2^{5/2}}\left(\frac{\Delta_\infty}{E_F}\right)^2$

An example: $(k_F a_i)^{-1} = 0$ and $T \approx T^*$



for $(k_F a_f)^{-1} = 2.6$

for $(k_F a_f)^{-1} = 3.2$

plateau $\frac{\Delta_\infty}{E_F} = 0.69^{+0.12}_{-0.16}$

theoret. value $\frac{\Delta_\infty}{E_F} = 0.73$

On the physical meaning of Δ_∞:

In our theory, the wave-vector distribution function $n(\mathbf{k})$ has the asymptotic behavior (for large $|\mathbf{k}|$)

$$n(\mathbf{k}) \approx \frac{(m\,\Delta_\infty)^2}{\mathbf{k}^4} \,,$$

to be compared with Shina Tan' result

$$n(\mathbf{k}) \approx \frac{C}{\mathbf{k}^4} \,,$$

where C is the "contact intensity" that enters several quantities of a Fermi gas in a universal way.

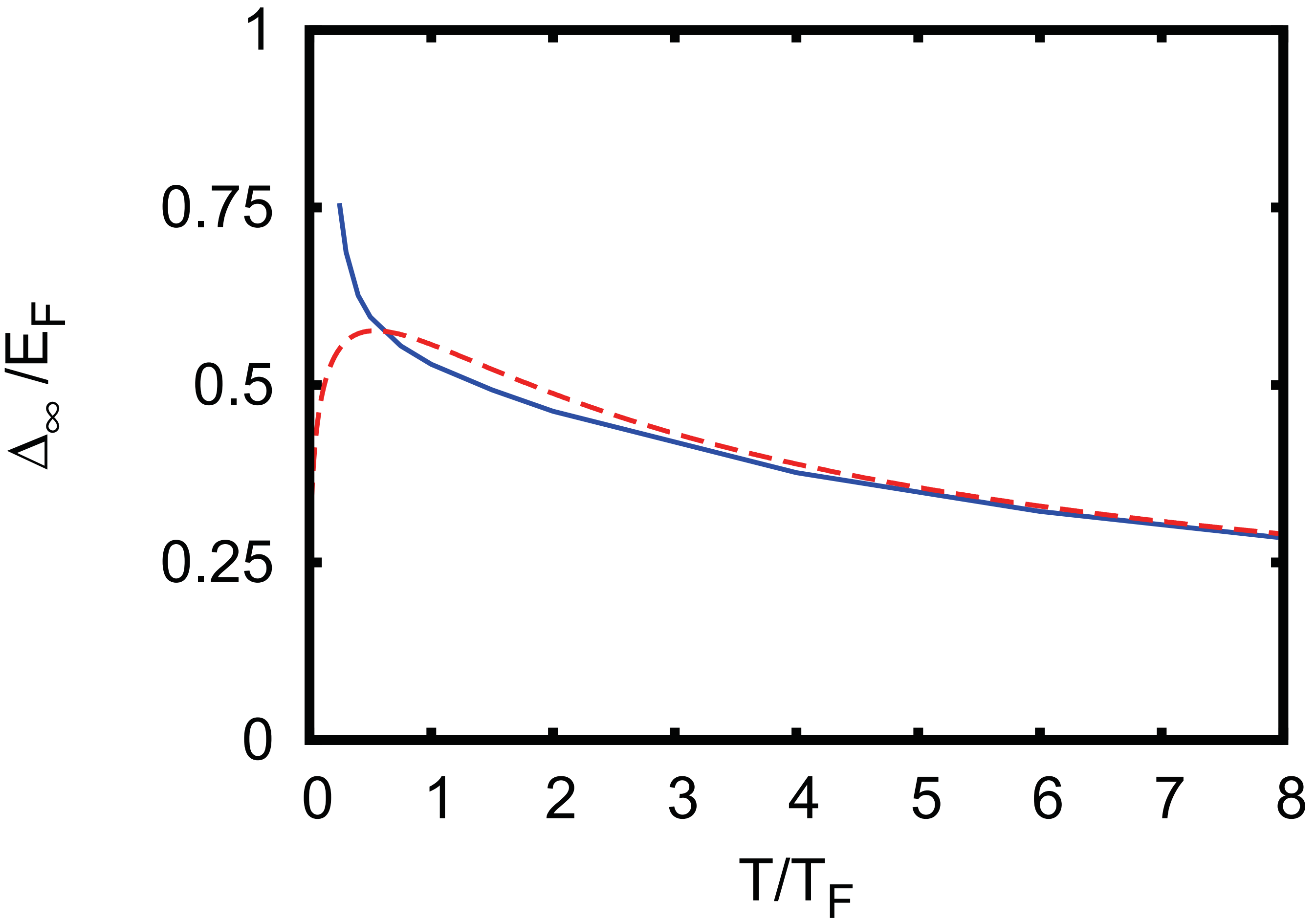
From our theory we identify $C = (m\,\Delta_\infty)^2$.

Δ_∞ throughout the BCS-BEC crossover:

- BCS regime : $\Delta_\infty = \frac{2\pi}{m}|a_i|n$ for $T \lesssim (ma_i^2)^{-1}$
- BEC regime : $\Delta_\infty^2 = \frac{4\pi n}{m^2 a_i}$ for $T \lesssim (ma_i^2)^{-1}$
- Unitarity regime for $T \to T_c^+$: $\frac{\Delta_\infty}{E_F} \simeq 0.75$

to be compared with the value $0.8 E_F$ of the "pseudo gap" extracted from single-particle spectral function.

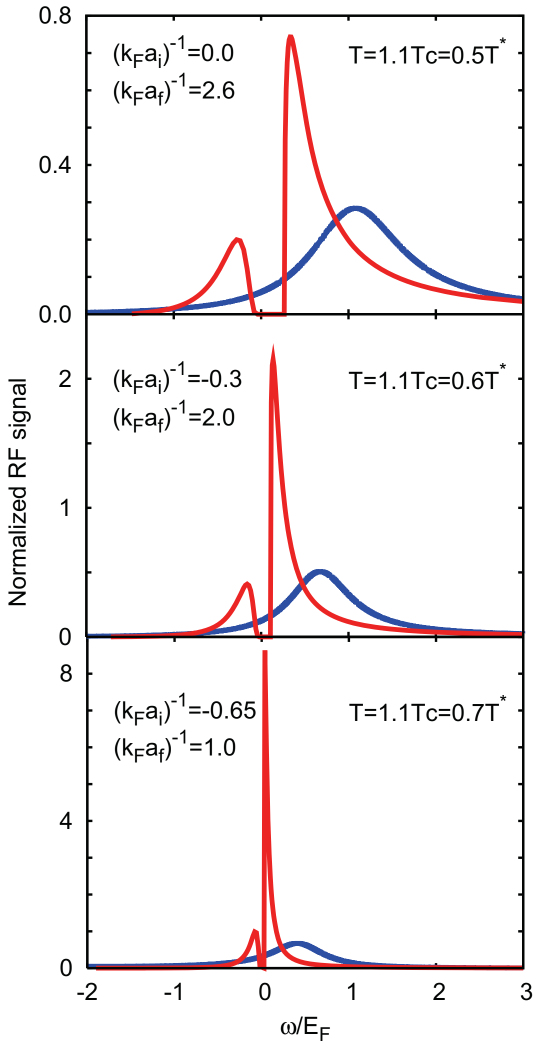
Δ_∞ vs T at unitarity:



numerical calculation

high-temperature expansion

Comparison of DOS+AL with BCS-RPA when $T_c \le T \le T^*$:



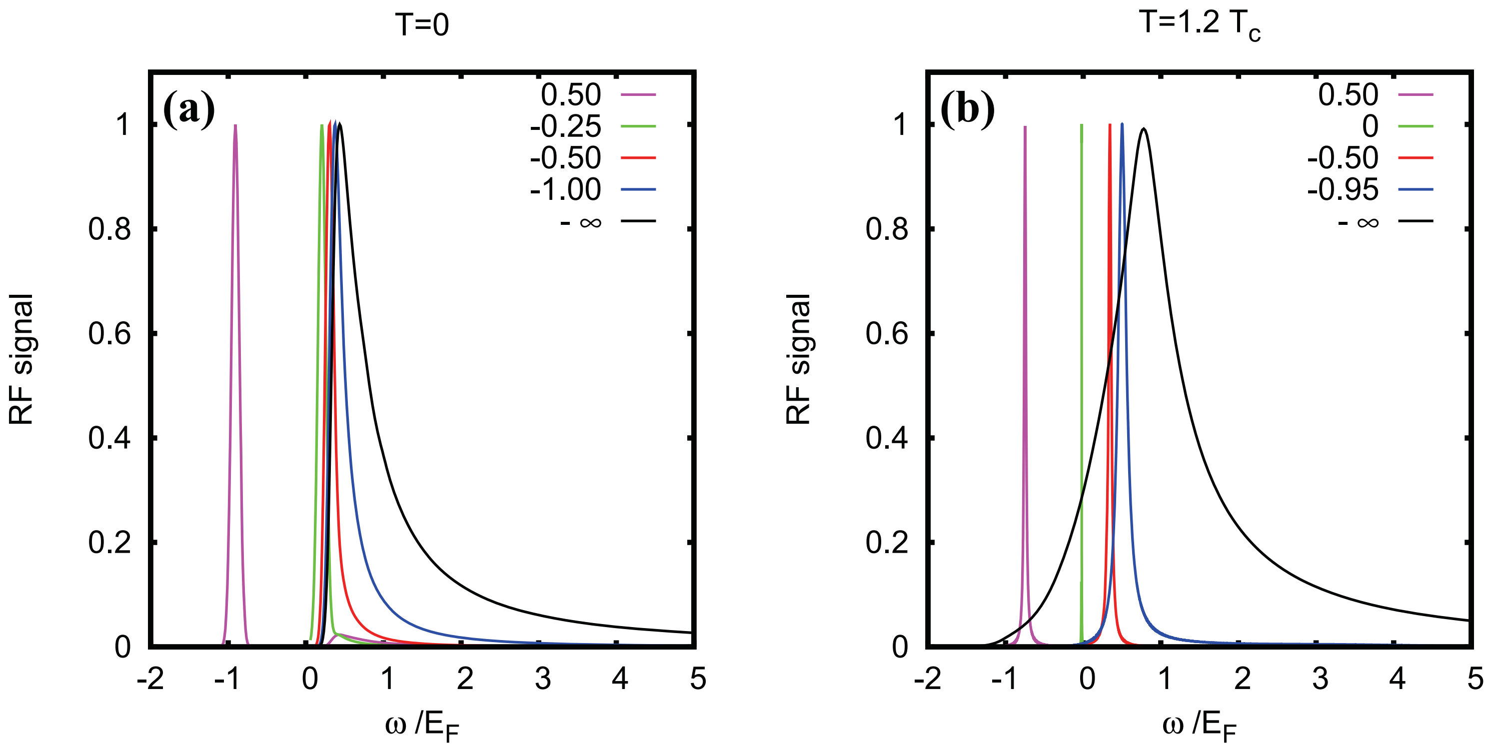
DOS+AL

BCS-RPA

(each curve with its own μ)

"Gedanken" experiment:

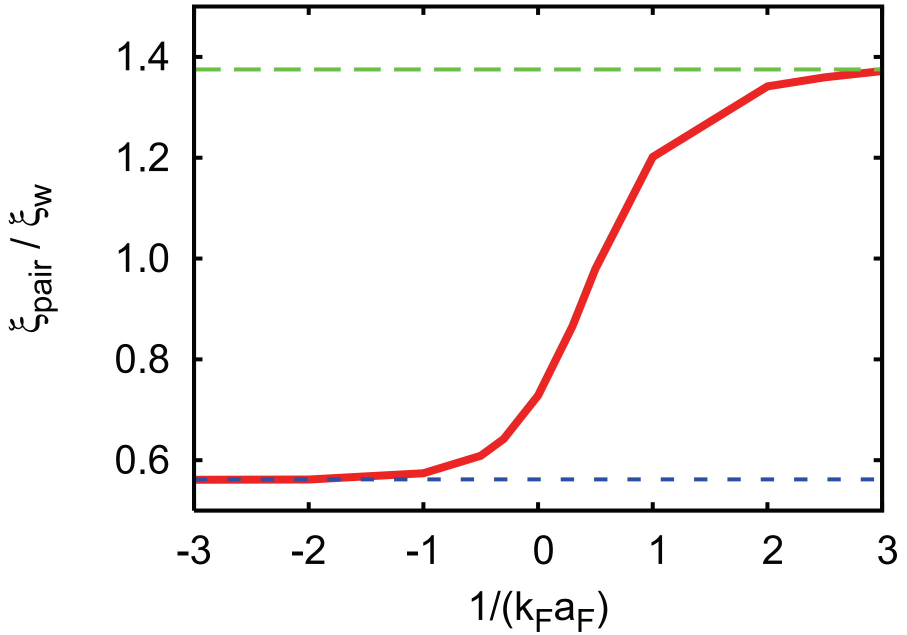
Once theory has been tested to work properly $\Longrightarrow$
do calculations where experiments cannot be done !



$(k_F a_i)^{-1} = 0$ $\qquad$ $(k_F a_f)^{-1}$ varies

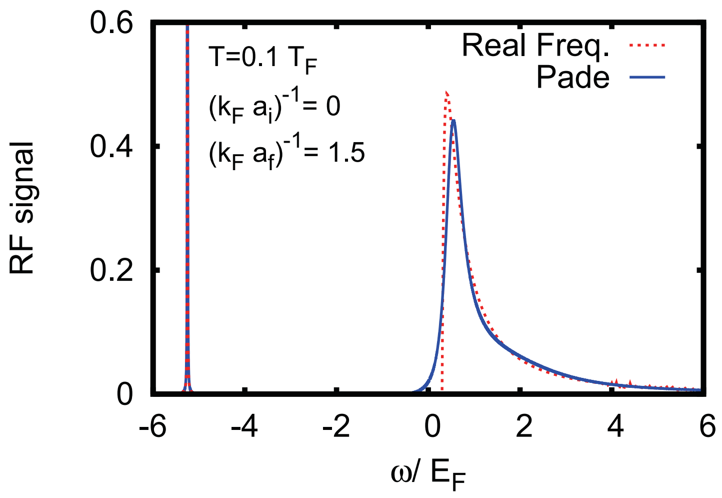
(a) BCS-RPA $\qquad$ **(b)** DOS+AL

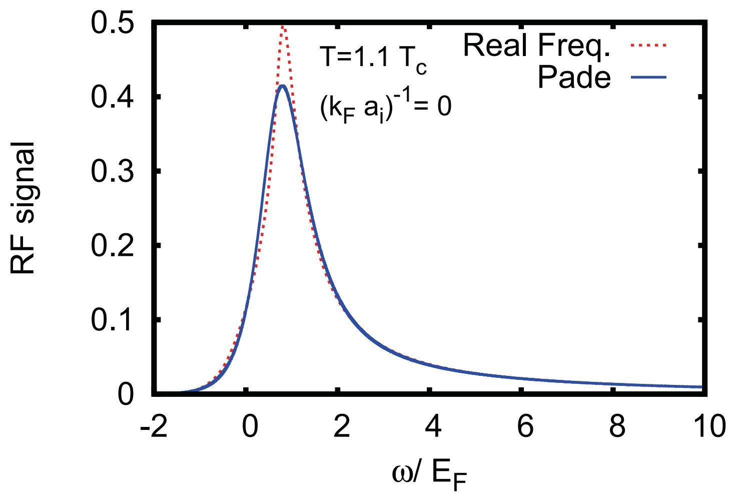
ξ_{pair} vs ξ_w within BCS bubble at $T = 0$ throughout the BCS-BEC crossover:



- Full width of half-maximum of RF continuum peak $= \dfrac{1}{2\, m\, \xi_w^2}$
- $\xi_{\mathrm{pair}}^2 = \dfrac{\int d\mathbf{r}\, \mathbf{r}^2\, g_{\uparrow\downarrow}(\mathbf{r})}{\int d\mathbf{r}\, g_{\uparrow\downarrow}(\mathbf{r})}$

Checking Padé approximants for RF spectra both below and above T_c:





BCS-RPA for $T < T_c$ DOS for $T_c < T$

In both cases, confront with an independent calculation made directly on the real-frequency axis.