Lecture 3 : Diagrams

Chapter 6 : Feynman diagrams for the lattice model

$$H = \sum_{\substack{k \in \mathcal{D}_L \\ \sigma = \uparrow,\downarrow}} \left(\varepsilon_k - \mu \right) c^+_{k\sigma} c_{k\sigma} + g_0 \sum_{\vec{x}} b^3 \, (\psi^+_\uparrow \psi^+_\downarrow \psi_\downarrow \psi_\uparrow)(\vec{x})$$

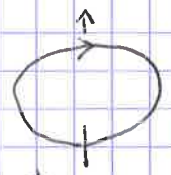
ε_k → e.g. $\frac{\hbar^2 k^2}{2m}$

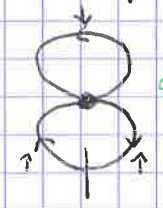
We want to compute one intensive quantity $Q(T, \mu_\uparrow, \mu_\downarrow)$

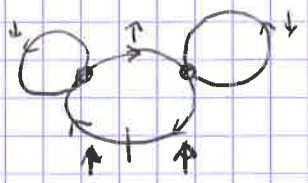
directly in thermodynamic limit

e.g. : $Q = n_\uparrow = \lim_{V \to \infty} \langle (\psi^+_\uparrow \psi_\uparrow)(\vec{0}) \rangle$ (EoS)

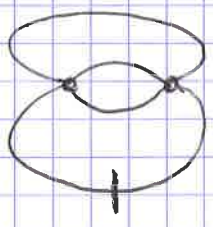
Expand Q in powers of g_0 — coefficients of expansion are conveniently represented by Feynman diagrams

$n_\uparrow =$  $\Leftarrow n^{(0)}_\uparrow \propto (g_0)^0$

$+$  $\Leftarrow g_0$

$+$ 

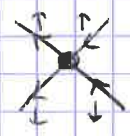
$+$ 

$+$  $\propto (g_0)^2$

$+ \ \ldots \ \Big\} \ O(g_0^3)$

Feynman rules :

1) Draw all connected diagrams using the building blocks :



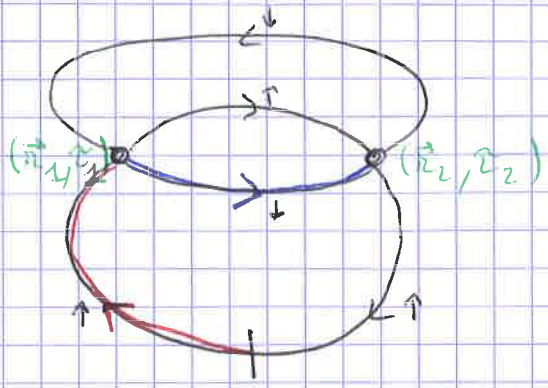
[because we have $(\psi^+_\uparrow \psi^+_\downarrow \psi_\downarrow \psi_\uparrow)(\vec{x})$ in H]

2) To compute the contribution to $n_\uparrow$ of a given diagram :

define $G_{0,\sigma}(\vec{x}, \tau) := \begin{cases} -\langle \hat{\psi}_\sigma(\vec{x}, \tau) \hat{\psi}^+_\sigma(\vec{0}, 0) \rangle & , \ \tau > 0 \\ +\langle \psi^+_\sigma(\vec{0}, 0) \hat{\psi}_\sigma(\vec{x}, \tau) \rangle & , \ \tau > 0 \end{cases}$

("propagator")

for example, the contribution to $n_\uparrow$ of the diagram :



is given by :

$$(-1)^{N_l}(-g_0)^2 \sum_{\vec{r}_1} b^3 \int_0^\beta d\tau_1 \sum_{\vec{r}_2} b^3 \int_0^\beta d\tau_2 \; G_{0\uparrow}(\vec{r}_1, \tau_1)\, G_{0\downarrow}(\vec{r}_2 - \vec{r}_1, \tau_2 - \tau_1) \cdot G_{0\uparrow}(\text{---})\, G_{0\downarrow}(\text{---})\, G_{0\downarrow}(\text{---})$$

N_l = # of internal loops = 1 here

∞

$$n_\uparrow = \sum_{N=0}^{\infty} a_N$$

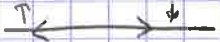
↳ sum of all order-N diag $\propto (g_0)^N$

"Bare diagrammatic scheme"

Note : Works for $\mathcal{V} = \infty$ because diagrams are connected. [≠ Det Diagrammic MC approach of Burovski et al and Goulko-Wingate]

Note : This can work only in the Normal phase

SF : $\langle \psi_\uparrow \psi_\downarrow \rangle \neq 0$ [see Neera Pauli' lecture on BCS theory]

hence we would need  "anomalous propagators"

In the continuum limit $b \to 0$:

each diagram $\to 0$

hence we would need to keep b finite (if we want to work with this bare scheme), and to go to very high order when b is very small → painful.

instead, we will use another diagrammatic scheme, see chapter 8.

Chapter 7 : Sign problem and sign blessing

in this Chapter, I will consider, for simplicity and concreteness, the Hubbard model : Hamiltonian of Chapter 6, with

$b = 1$, $g_0 = U > 0$ $\quad \varepsilon_k = -2t \sum_{i=1}^{d} \cos(k_i)$

[see J. Thijssen's lectures]

The (fermionic) sign problem : in Monte Carlo simulations, one typically computes

$$\frac{1}{I} \sum_{i=1}^{I} c_i \xrightarrow[I \to \infty]{} \bar{c} = \text{physical result}$$

c_i : random numbers, can be >0 or <0, >0 and <0 ones nearly cancel each other due to fermionic antisym.

$$\left[\frac{\left| \sum_{i=1}^{I} c_i \right|}{\sum_{i=1}^{I} |c_i|} \xrightarrow[I \to \infty]{\text{rapidly}} 0 \right]$$

$\Rightarrow$ need long CPU time (large I) to have (statistical error) $\ll \bar{c}$

1) Finite-volume methods

simulate finite-size system, volume V

then try to extrapolate $V \longrightarrow \infty$ (Thermodynamic limit)

- Auxiliary Field Quantum Monte Carlo :

  statistical error $\varepsilon_{stat} \sim e^{\#\beta V}$ (except at half-filling where there is no sign problem)

  prohibitive $\longrightarrow$ one usually makes approximations ("constrained path") based on a trial wavefunction to avoid the sign problem.

  For a recent achievement, see arXiv:1701.00054 : Stripe order (comparing different trial wavefunctions and to other methods)

- Cluster DMFT : $\varepsilon_{stat} \sim e^{\#\, v_{cluster}}$

  $v_{cluster} \to \infty$ extrapolation challenging.

2) ∞ - Volume approach — usually called Diagrammatic MC

[see arXiv : 0802.2923 — first demonstration
[CDet] : 1612.05184 — a new algorithm ←
1809.04651 — yet another algorithm, impressive results for the electron gas]

$$Q = \sum_{N=0}^{N_{max}} a_N$$

$$MC : \left[a_N = \lim_{I \to \infty} \frac{1}{I} \sum_{i=1}^{I} c_i \right]$$

sign problem : $\left[\left| \sum c_i \right| \ll \sum |c_i| \right]$

$\Rightarrow$ $t_{CPU}(N)$ ↗ quickly

[$e^{\#N}$ in best case]

but also sign blessing :

$$|a_N| \ll \#\text{ of diagrams} \sim N!$$

due to near cancellations between diagrams that occur due to fermionic antisymmetry.

Series can even converge $|a_N| \sim e^{-\#N}$ ←

This happens for $\frac{U}{t} \leq 4$, for a diagrammatic scheme slightly more advanced than the bare scheme (namely a scheme where tadpole diagrams are resummed) and already allows to get state-of-the art results [see arXiv : 0907.0863 and [CDet]].

Summarizing : { • (exponentially) expensive to access large N (↓ for CDet)
• but pays exponentially well, because

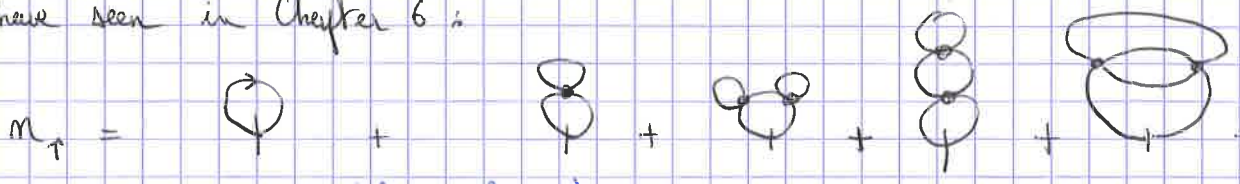
net result : $t_{CPU} \sim \frac{1}{(\varepsilon_{stat+trunc})^2}$ (polynomial!)

[arXiv : 1703.10141]

= Best possible scaling for MC.
Note : no fundamental limitation due to some "NP-hardness"..

Chapter 8 : Feynman diagrams for the ~~Zero Range Model~~ (in the Zero-Range Model)

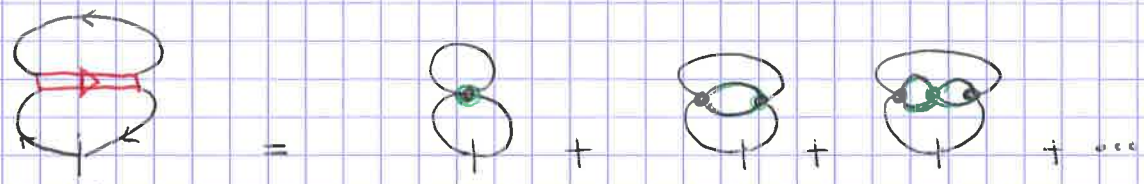
We have seen in Chapter 6 :



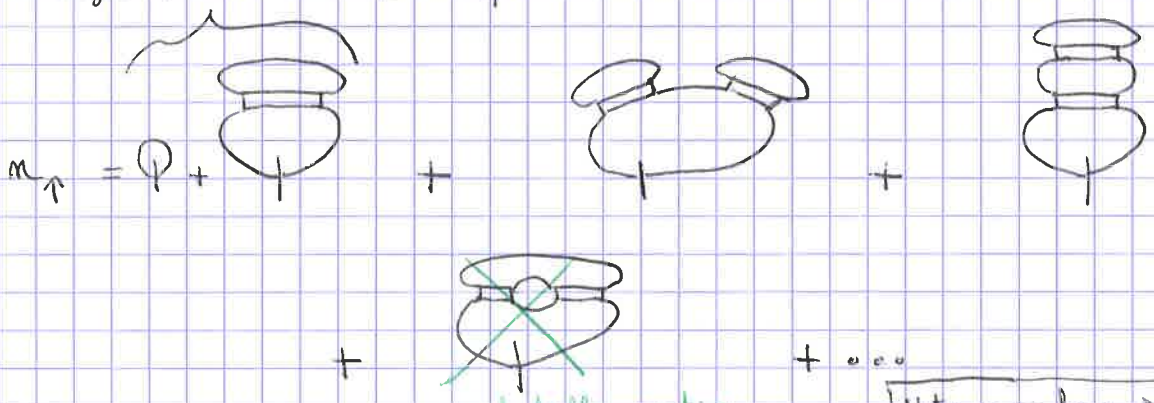
(bare scheme)

Define

$$-\Gamma_0(\vec{x},\tau) := -g_0 \cdot \frac{\delta_{\vec{x},\vec{0}}}{b^3} \cdot \delta(\tau) + (-g_0)^2 (G_\uparrow G_\downarrow)(\vec{x},\tau) + \dots$$



Nozières Schmitt-Rink : $n_\uparrow = 0$.



avoid double-counting

"Ladder scheme"

Note : we have redrawn the diagrams when going from Bare to Ladder scheme. A priori : unjustified. But we will justify it later

$$n_\uparrow = \sum_{N=0}^{\infty} a_N^{(\text{Ladd})}$$

→ order N ≡ contains N Γ_0-lines.

Γ_0 is well-defined in the limit $b \to 0$.

→ we can directly deal with the ZRM.

Problem : series diverges

Remark : in QED, diagrammatic series are of the form $\sum_N a_N \cdot \alpha^N$

Series diverges (for any α) [Dyson's argument (1952) about the instability of the vacuum if α is made negative. Confirmed by Itzykson-Zuber-Parisi-Balian and Bogomolny-Fateyev who obtained/conjectured : $|a_N| \sim (\frac{N}{2})!$]

But $\alpha \ll 1$ ⇒ series behaves as a convergent series if truncated at N_{max} not very large

[if $N_{max} \lesssim \frac{2e}{\alpha^2} \simeq 2e \cdot 137^2$]

→ for all practical purpose, behaves as a rapidly convergent series. → Results tested with ~10 digits accuracy (experiments of Bireben + Gabriele's groups)

Back to resonant Fermi gas :

in strongly correlated regime, no small expansion parameter.

$\sum_{N=0}^{N_{max}} a_N$ strongly depends on N_{max}, $\forall N_{max}$.

① Does the diagrammatic series "$\sum_{N=0}^{\infty} a_N$" mean anything mathematically ? ② if so, is it useful to compute the EoS accurately and reliably ?

Answer : Yes !

We will :

① To give a mathematical meaning to "$\sum a_N$" :

Define $Q(z)$, a function of a formal complex parameter z, such that :

- The Taylor series of $Q(z)$ for $z \to 0^+$ is $\sum a_N z^N$, i.e. : $\lim_{\substack{z \to 0 \\ z \in \mathbb{R}^+}} \frac{1}{N!} \frac{d^N Q(z)}{dz^N} = a_N$
- $Q(z=1) = n_\uparrow$ (= the exact physical quantity we want to compute)
- $Q(z)$ is analytical in a domain that contains $(0, 1]$.

② Design a "resummation method" $\mathcal{R}$ such that

$\mathcal{R}(a_0, a_1 \cdots a_{N_{max}}) \xrightarrow[N_{max} \to \infty]{} Q(1) = n_\uparrow$.

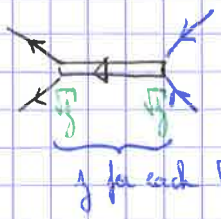
③ Compute numerically (for $N_{max} \leq 9$) and check the convergence and compare with experiment

[with Rossi, Ohgoe & Van Houcke, arXiv : 1802.07717]

How :

For ① : idea :

• interpret :  as the propagator for some boson (a pair)



1 boson ⟶ 2 fermions
⟵

ζ for each Γ_0

• define a model $\mathcal{N}(\zeta)$

(by an action $S^{(\zeta)}[\varphi_0, \xi]$ ← Grassmann field (fermionic) ; ← Complex field (bosonic))

s.t. • $\mathcal{N}(\zeta=1) \Longleftrightarrow$ RFG

↑ integrate out boson field

• Base scheme for $\mathcal{N}(\zeta)$ (i.e. expansion in ζ) $\Longleftrightarrow$ (Ladder scheme for RFG

Note : Our construction of $\mathcal{N}(\zeta)$ is non-perturbative. We do not rely on the Base scheme and its reshuffling of the order of summation to get the ladder scheme as presented in ~~Chapter 6~~ the beginning of this chapter.

For ② : General question :

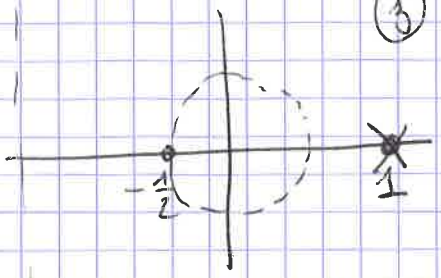
$\sum a_N \zeta^N$ | Taylor $\zeta \to 0^+$ $\{\varphi(\zeta)\}$

$(a_N) \xrightarrow[\text{unique ? compute ?}]{?} \varphi(\zeta=1)$

Excursion : if $\varphi(\zeta)$ analytic at $\zeta=0$ (and hence in a disk around $\zeta=0$)

→ simple example : $\varphi(\zeta) = \dfrac{1}{1+2\zeta}$

③



$= \sum_{N=0}^{\infty} (-2)^N \cdot \zeta^N$ for $|\zeta| < \frac{1}{2}$

analytic continuation outside disk $\{|\zeta| < \frac{1}{2}\}$

• unique

• computed : $\varphi(1) = \lim_{\varepsilon \to 0^+} \sum_{N=0}^{\infty} (-2)^N e^{-\varepsilon N \ln N}$

$= \dfrac{1}{3}$

→ This applies to Fermi polaron ($N_\downarrow = 1$, $N_\uparrow \to \infty$, $\upsilon \to \infty$ $n_\uparrow$ fixed)

Back to RFG : Lindelöf works well for E.S and $\mathcal{G}$
(Van Houcke et al. 2012-13)

but more recently we found (R. Rossi PhD Thesis) :

$$|a_N| \sim (N!)^{1/5}$$

⇒ $Q(z)$ not analytic at $z=0$

⇒ are we doomed ?

is the mapping $(a_N) \longrightarrow Q(z=1)$ non-unique ?

$$\tilde{Q}(z) = Q(z) + \text{cst} \cdot e^{-\frac{1}{z}}$$

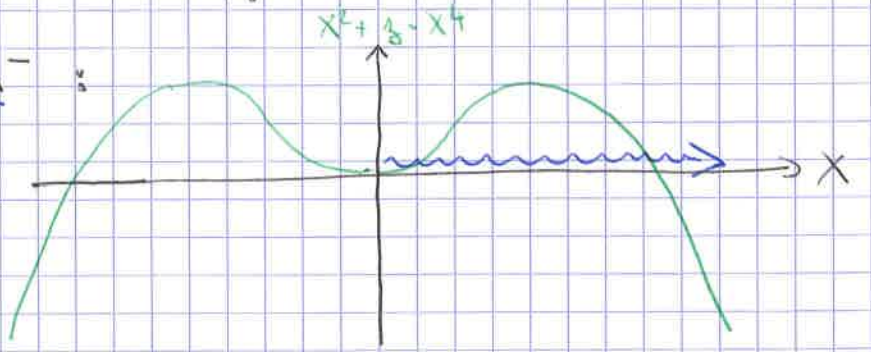
($\tilde{Q}$ and Q: same Taylor series (a_N))

Excursion : anharmonic oscillator

$$H = \hat{P}^2 + \hat{X}^2 + z \cdot \hat{X}^4$$

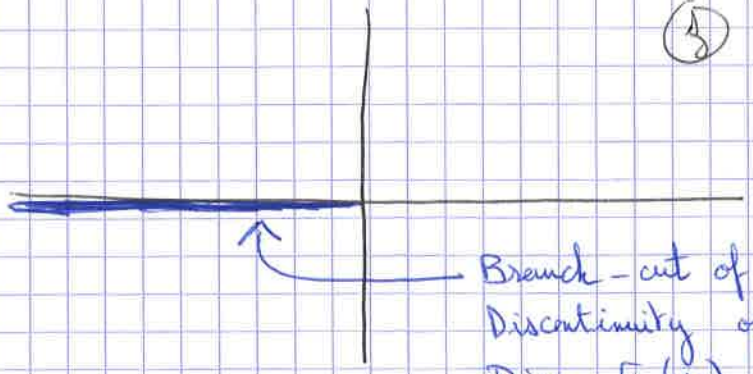
Ground-state energy : $E_0(z) = ?$

if $z \in \mathbb{R}^-$:



Ground-state becomes unstable

decay rate $\Gamma \propto \text{Im}\, E_0(z)$



Branch-cut of $E_0(z)$

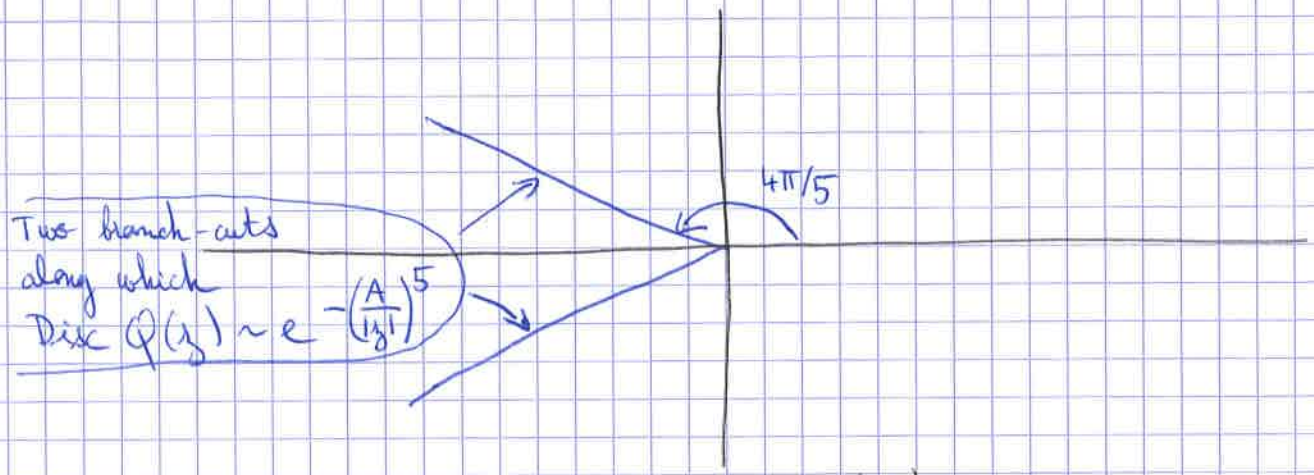
Discontinuity of $E_0(z)$ through the cut

Disc $E_0(z) \sim \Gamma \sim e^{-\frac{A}{|z|}}$ for $z \to 0$, $z \in \mathbb{R}^-$.

No $e^{-\frac{1}{g}}$

It was shown that $E_0(1)$ can be obtained from (a_N) using a conformal-Borel resummation method.

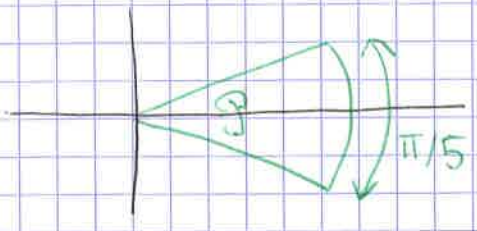
For the RFG, we find:



$Q(g=1)$ can be obtained from (a_N) by an appropriate (generalized) conformal-Borel resummation method.

To justify this, we use Nevanlinna's theorem (1919) which basically states that this holds provided

$$\frac{1}{N!}\left|\frac{d^N Q(g)}{dg^N}\right| < (N!)^{1/5} \cdot \alpha t^N \quad , \forall g \in \mathcal{P} \qquad (*)$$



Notes: $Q(g) = e^{-\frac{1}{g}}$ violates $(*)$, as it should.

Results

So far, $a = \infty$, $\mu_\uparrow = \mu_\downarrow$, normal phase.

At low $\frac{T}{T_F}$, the ladder scheme is not applicable any more, and we instead used a "bold scheme" (self-consistent). The above steps to justify applicability of a conformal-Borel resummation method remain, although some details of the derivations were more hand-waving.

Our main findings are:

- For the Equation of State, we confirm our 2012 data, now with error-bars that are smaller ($\sim 10^{-4}$ at $\frac{T}{T_F} = 2$, $\sim 10^{-2}$ at $\frac{T}{T_F} \simeq 0,2$) and much more reliable

((in 2012 we used Lindelöf resummation, which is not applicable mathematically as we now ~~~~ know — there was a systematic error, which happened to be small due to the smallness of $\frac{1}{5}$: $(N!)^{-1/5}$ does not grow much faster than $e^{\#N}$ for $N \leq 9$))

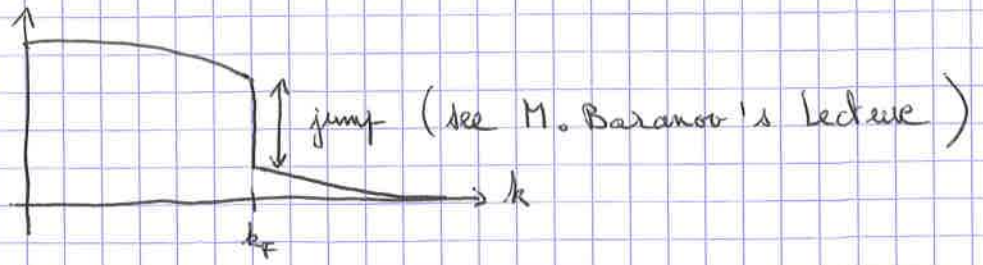
We resolve the discrepancy about the 4th virial coefficient mentioned in F. Chevy's Lecture b_4 V: The Ende-Carlin value appears correct, but requires very high accuracy and high enough $\frac{T}{T_F}$ to be seen in the EoS.

[arXiv: 1802.07717, data in Suppl. Mat.]

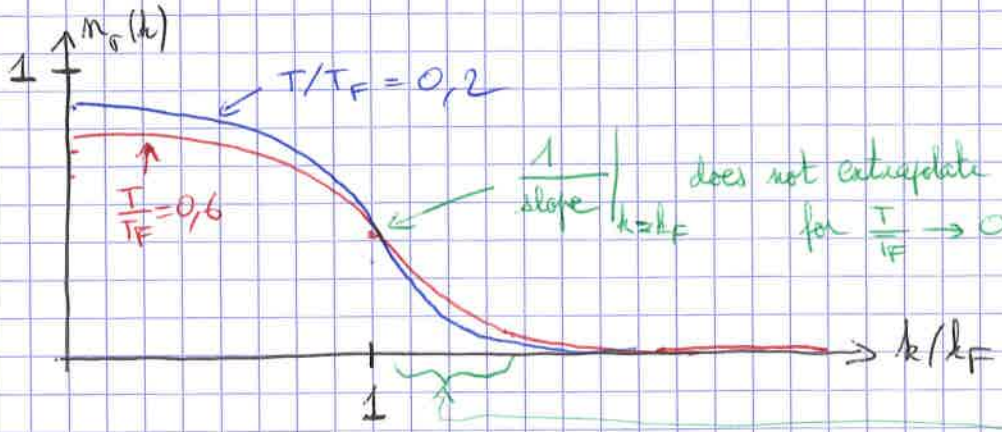
- For C and $n_\sigma(k)$ [arXiv: 1303.6245 v3]

1) $n(k)$ does not follow Fermi-liquid theory:

For a Fermi-liquid in the $T \to 0$ limit:



our data :



2) $\frac{\mathcal{E}}{k_F^4}$ decreases slowly : only ~ 10% change from $\frac{T}{T_F} = 0,2$ to 0,6.

This appears to result from two effects that nearly cancel out :