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FACULTÉ DES SCIENCES D'ORSAY
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LPTMS Laboratoire de Physique Théorique et Modèles Statistiques
LPS ORSAY
PROJET FINANCÉ PAR L'ANR - PROJECT FUNDED BY THE ANR

Coexistence and phase separation of pairs and fermions in a one-dimensional model with pair-hopping

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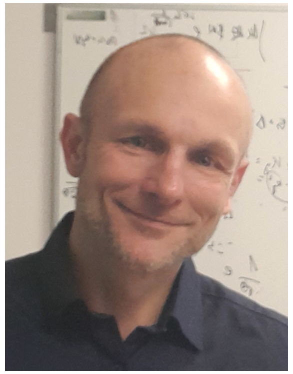


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Quantum 2021 : Dynamics and local control of impurities in complex quantum environments

Monday August 30rd

Outline

References for this work: Phys. Rev. Lett. **126**, 206805 (2021) and arXiv:2107.11132

see references inside for many cited and relevant works

General context

pairing in one-dimensional system

the Ruhman-Altman model

Pairing and two-fluid model in a spinless pair-hopping model

Phase diagram and limiting cases

Realization of a coexistence phase of pairs and fermions

Extensions

Effect of nearest neighbour interaction

Phase separation of pairs and fermions

Pairing in 3D

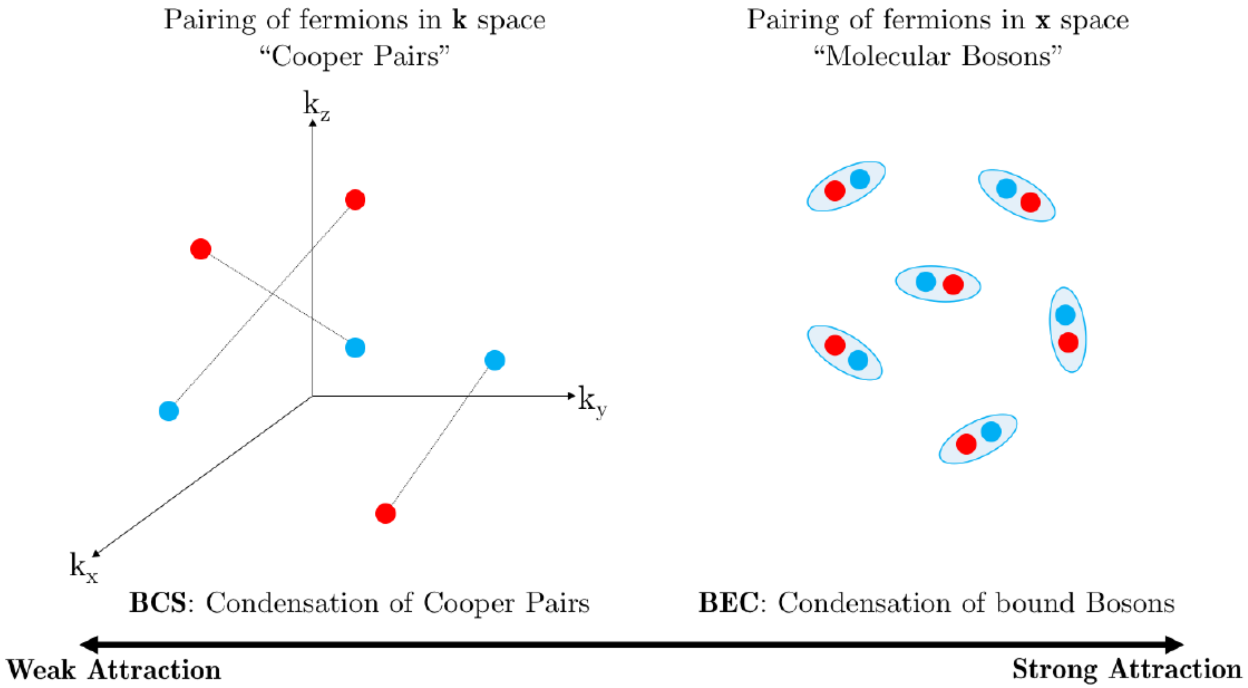
How to pair two fermions into a boson ?

BCS theory historical picture : opposite spins, opposite momenta

$$H = \sum_{\mathbf{k}\sigma} \xi_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \frac{1}{N} \sum_{\mathbf{k}\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} c^{\dagger}_{\mathbf{k}\uparrow} c^{\dagger}_{-\mathbf{k}\downarrow} c_{-\mathbf{k}'\downarrow} c_{\mathbf{k}'\uparrow}$$

Cooper pair

Molecule formation
and BCS – BEC crossover
driven by the range of
interaction



Pairing in one-dimensional systems

- **Pairing particles with an internal degree of freedom**

Hubbard-like model for spin-1/2 fermions
=> opening of a single particle gap, BKT transition towards a Luttinger liquid of pairs,
all fermions are involved in pairs

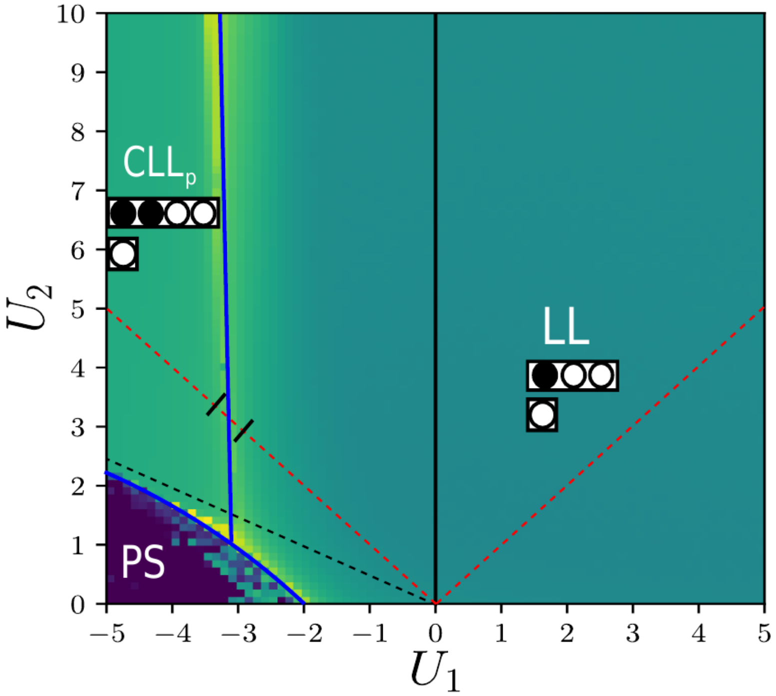
larger « molecules » possible using either mass imbalance and higher spins : trimers, etc...

- **More recently : studies of pairing of spinless fermions**

first strategy : neighbouring attraction to favor pairing,
next-nearest neighbour repulsion to fight phase separation

$$H = \sum_{j=1}^{L} \left[-t(\hat{c}_j^\dagger \hat{c}_{j+1} + h.c.) + U_1 \hat{n}_j \hat{n}_{j+1} + U_2 \hat{n}_j \hat{n}_{j+2} \right]$$

second strategy : pair-hopping term, studied a lot for
spinful fermions in the 2000s



Ruhman & Altman model and results

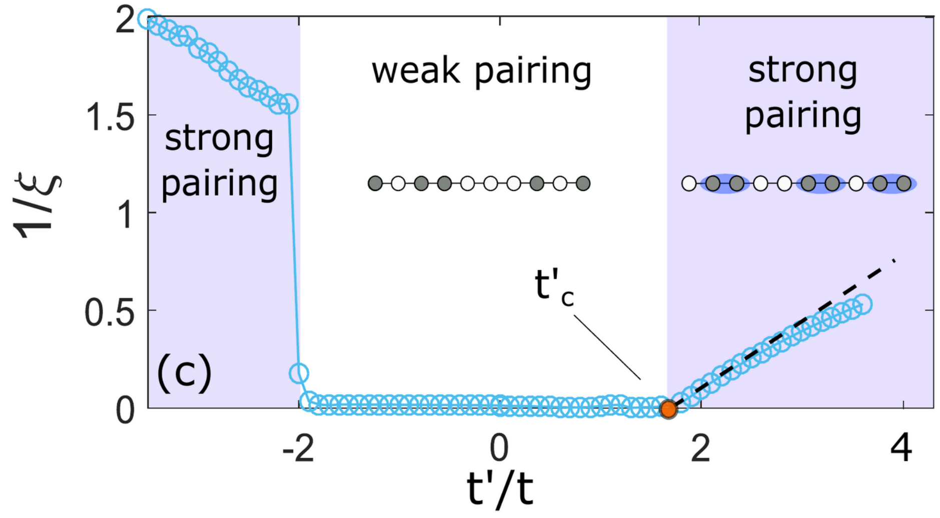
Phys. Rev. B **96**, 085133 (2017)

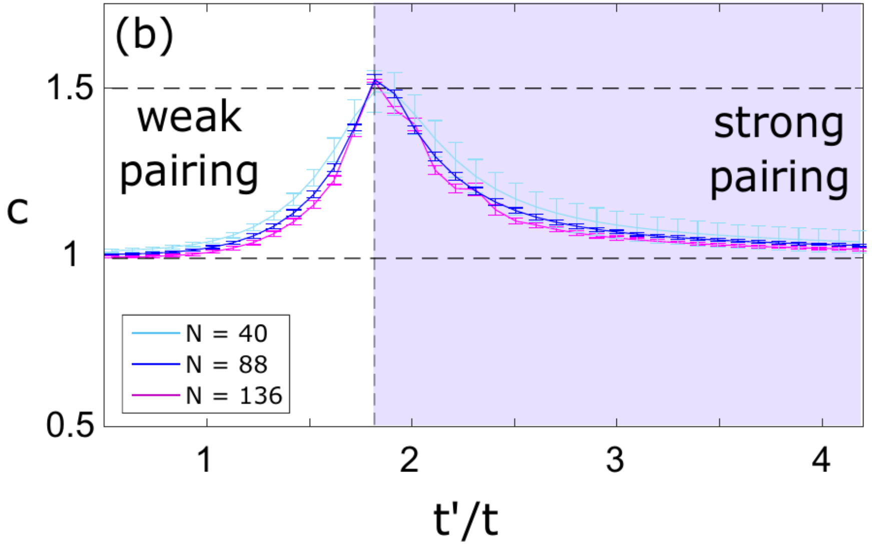
- **Their motivation** : looking for a 1D BCS-BEC-like model with both a weakly paired phase and a strongly paired phase of spinless fermions

- **The model** : spinless fermions with pair hopping

$$H = -\sum_{x=1}^{N}[t\,\psi^{\dagger}_{x+1}\psi_x + t'\,\psi^{\dagger}_{x+1}\psi^{\dagger}_{x}\psi_x\psi_{x-1} + \mathrm{H.c.}]$$

- Find a transition with an **emergent Majorana degree of freedom** from central charge *c* =1+**1/2** => possible application to topological computing etc… (beware of sign error in *t'* !)



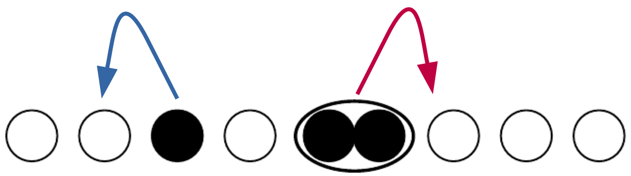


- Propose a setup with an inhomogenenous chain to create Majorana degrees of freedom at the interfaces between the domains

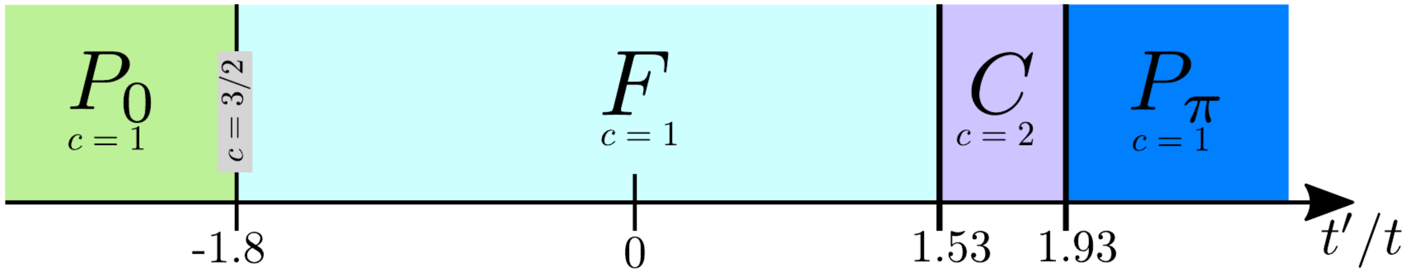
Pairing and two-fluid model in a spinless pair-hopping model

Chain of size *L* with spinless fermions with density $n = 0.25$

$$H = -t\sum_j \left[c_j^\dagger c_{j+1} + \text{h.c.}\right] - t'\sum_j \left[c_{j+1}^\dagger c_j^\dagger c_j c_{j-1} + \text{h.c.}\right]$$



Phase diagram $\tau = t'/t$



F : regular fermionic Luttinger liquid
P_0 : paired phase with k =0 pairs
P_π : paired phase with k =π pairs
C : coexistence phase with
both k =π pairs and unpaired fermions

c is the central charge

Pairs with finite momentum

- At large $\tau = t'/t$, the pairing term leads and favors pairing by kinetic energy gain.

- Depending on the sign of t', pairs condense at k =0 or k =π

- **Interpretation through a simple effective model**
  restrict the Hilbert space to neighbouring pairs of number N_b = $N/2$
  and maps to XY model : $|\bullet\bullet\rangle \rightarrow |\uparrow\rangle, |\circ\rangle \rightarrow |\downarrow\rangle$
  a subtlety : the size of the effective chain is now $L_b = L - N_b$

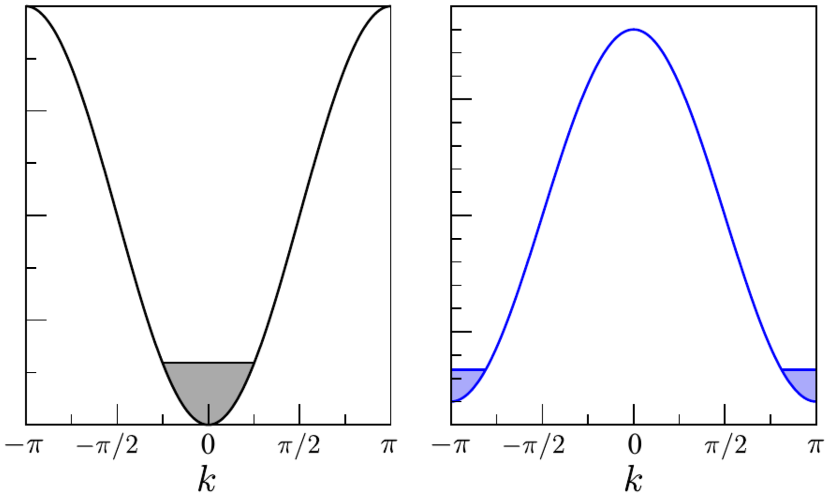
$$\hat{H} = t' \sum_{j=1}^{L_b} \left[\hat{\sigma}_j^+ \hat{\sigma}_{j+1}^- + H.c.\right]$$

- **Dispersion relation for pairs** : $\varepsilon_p(k) = 2t' \cos(k)$

- H is invariant un the unitary transformation $c_j \rightarrow e^{i\frac{\pi}{2}j} c_j$

$$c_j c_{j+1} \rightarrow (-1)^j i c_j c_{j+1}$$

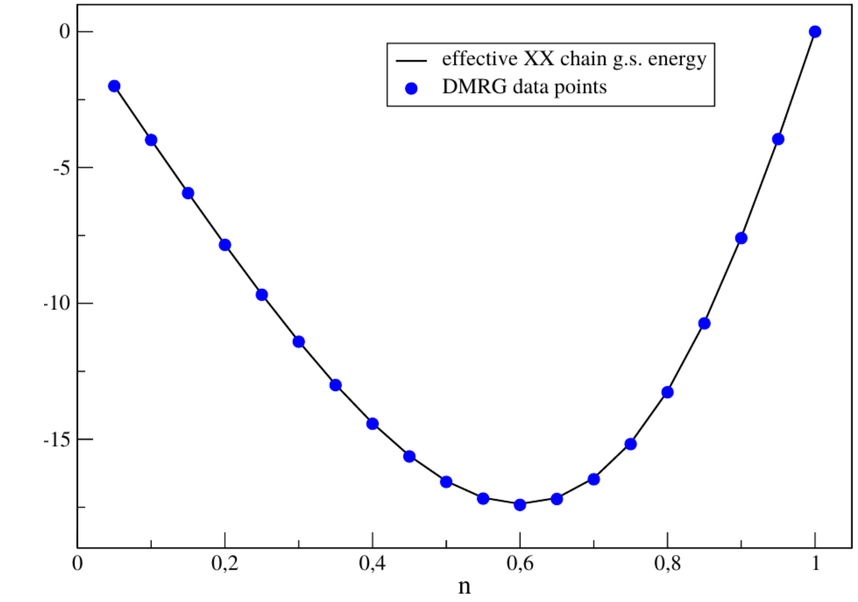
  the two phases P_0 and P_π are connected by a phase shift $k \rightarrow k+\pi$



Comparison with numerics

- **Ground-state energy** of effective model vs DMRG for t =0

$$e_{\rm eff} = \frac{1}{L}\sum_{|k|<\pi\frac{N_b}{L_b}} \varepsilon_p(k) = -\frac{2|t'|}{\pi}\left(1-\frac{n}{2}\right)\sin\left(\frac{\pi n}{2-n}\right)$$



- **Pair correlations**

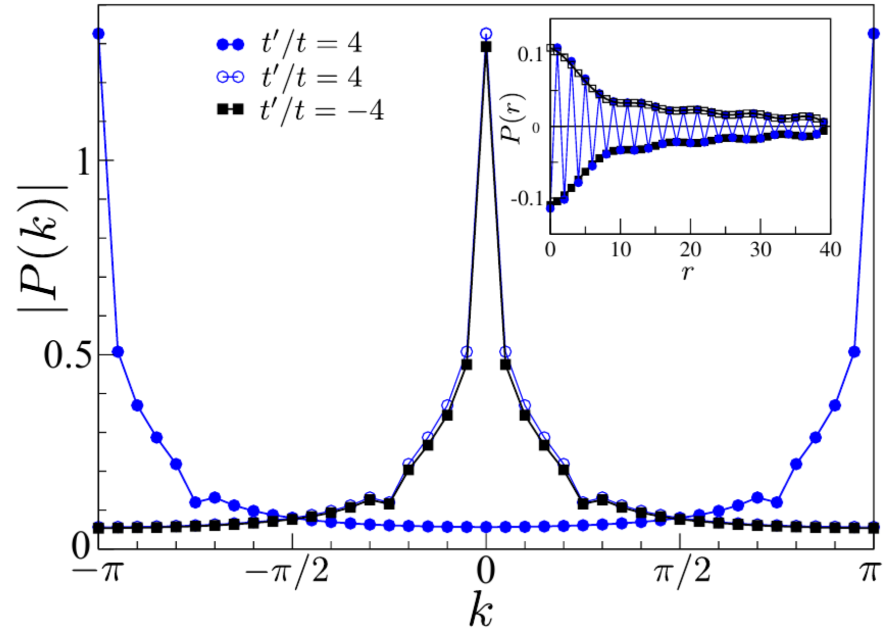
  ~ Green's function of hard-core bosons

$$P(r) = \langle c^\dagger_{\frac{L}{2}} c^\dagger_{\frac{L}{2}+1} c_{\frac{L}{2}+r} c_{\frac{L}{2}+r+1}\rangle$$

they essentially differ only by a factor (-1)^r

- **Pair structure factor**

$$P(k) = \frac{1}{L}\sum_{j,j'} e^{ik(j-j')}\langle c^\dagger_j c^\dagger_{j+1} c_{j'} c_{j'+1}\rangle$$



Observables in the paired phases

- **Local observables**

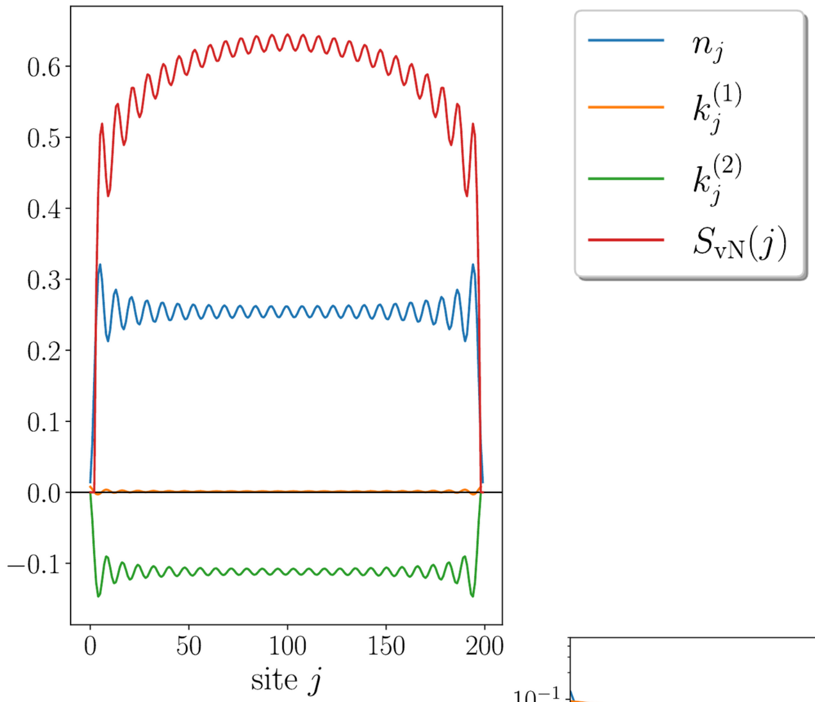
density $n_j = \langle \hat{n}_j \rangle$

kinetic energies

$$k_j^{(1)} = -\langle \hat{c}_j^\dagger c_{j+1} + H.c. \rangle,$$

$$k_j^{(2)} = -\langle \hat{c}_j^\dagger \hat{c}_{j+1}^\dagger \hat{c}_{j+1} \hat{c}_{j+2} + H.c. \rangle;$$

entanglement entropy profile $S_{\mathrm{vN}}(j)$

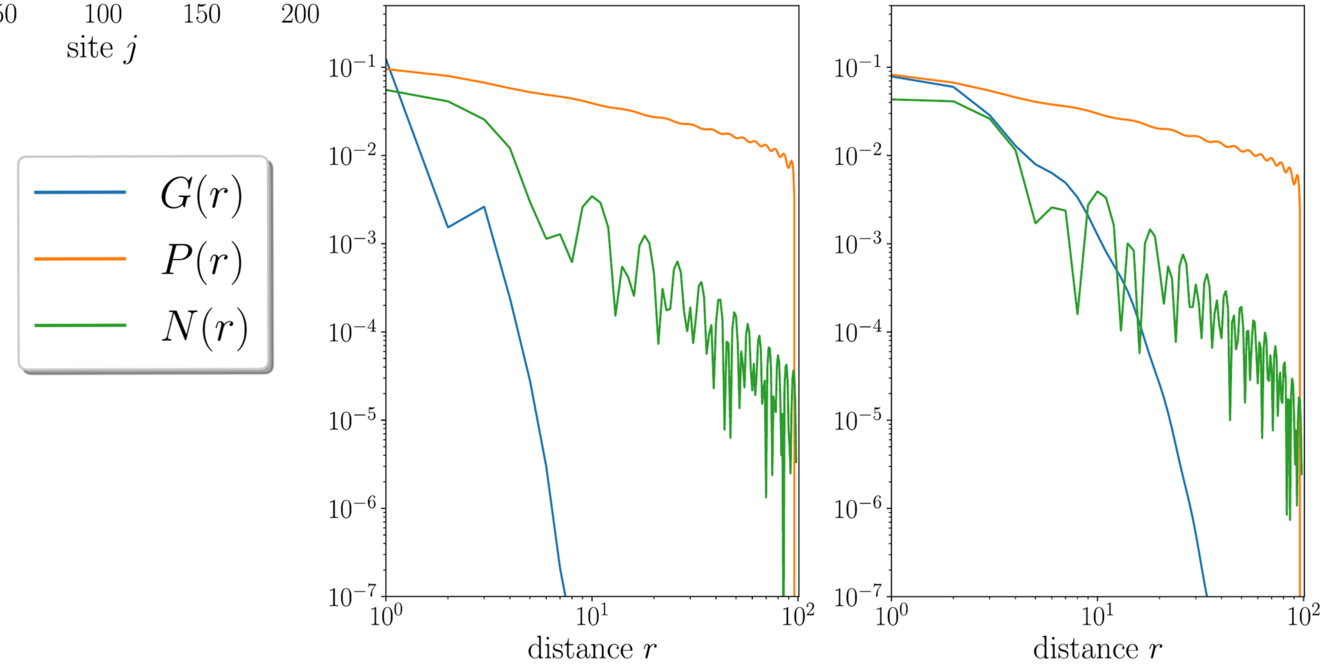


- **Correlations**

single-particle $G(r) = \langle \hat{c}_j^\dagger \hat{c}_{j+r} \rangle$

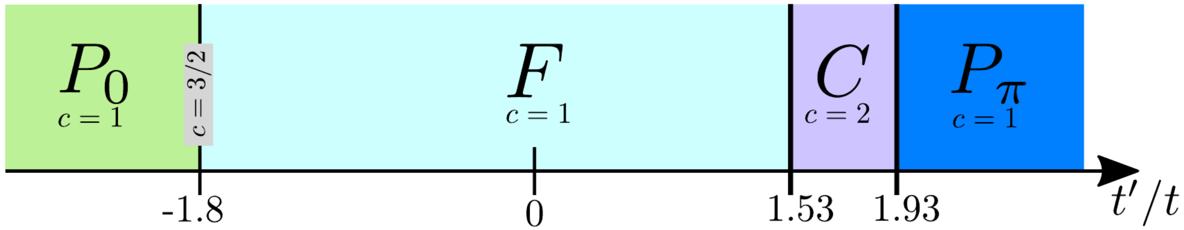
pair $P(r) = \langle \hat{c}_i^\dagger \hat{c}_{i+1}^\dagger \hat{c}_{i+r} \hat{c}_{i+r+1} \rangle$

density $N(r) = \langle \hat{n}_j \hat{n}_{j+r} \rangle - \langle \hat{n}_j \rangle \langle \hat{n}_{j+r} \rangle$



- **single mode *c* =1 Luttinger liquids with single-particle gap and strongly localized pairs**

The fermionic phase

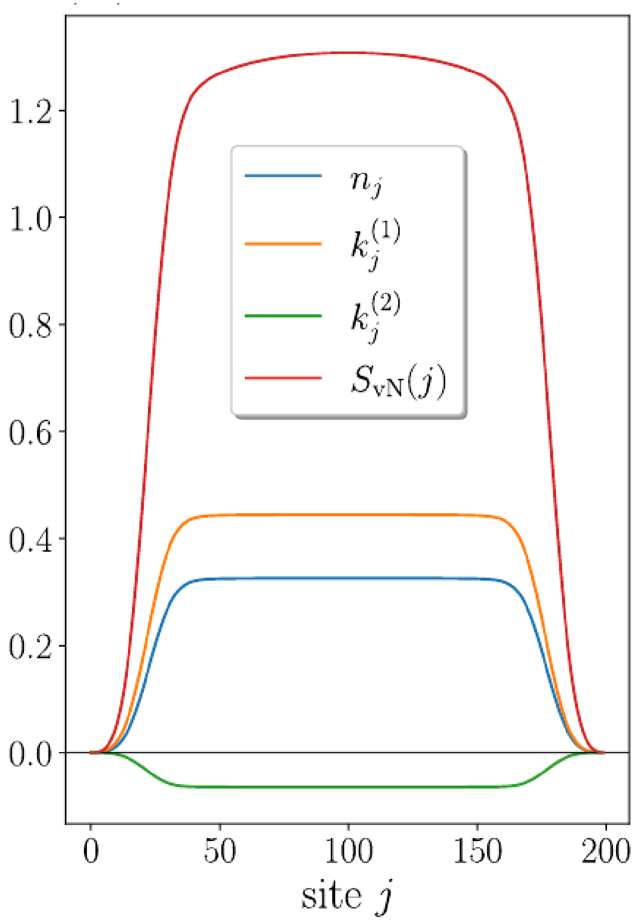


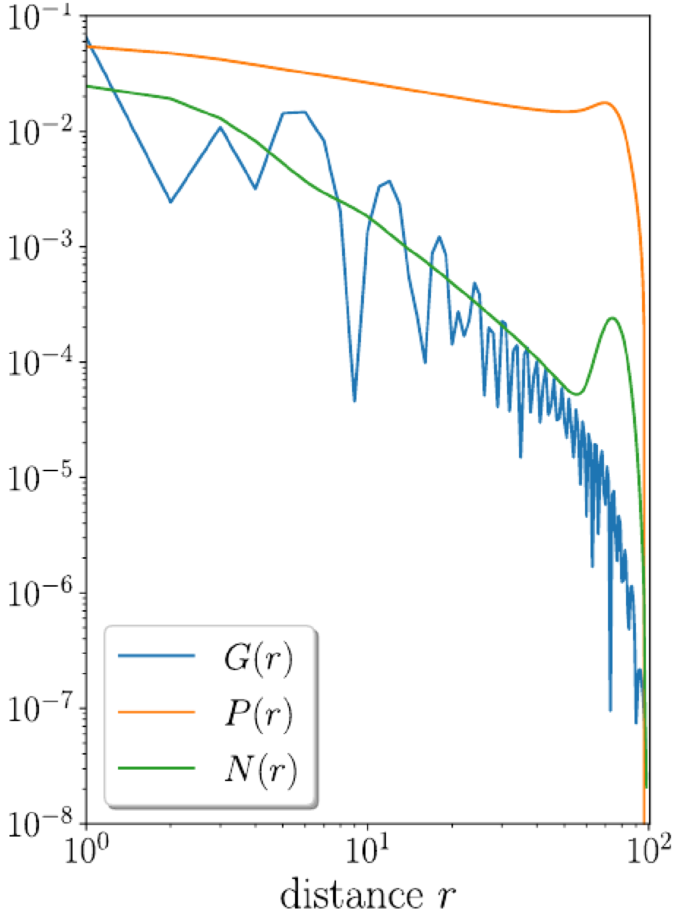
- **A regular single-mode *c* =1 Luttinger liquid** with gapless single-particle excitations

  if the Luttinger parameter *K* is large enough, pairing fluctuations can dominate

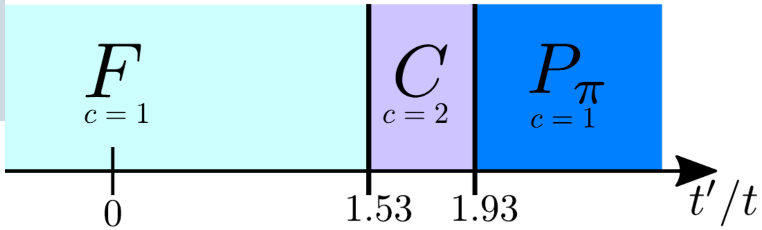
- **Transition from *F* => *P₀***

  after Ruhman & Altman
  the transition has an extra Majorana degree of freedom leading to a
  c = 1 + 1/2 = 3/2
  central charge



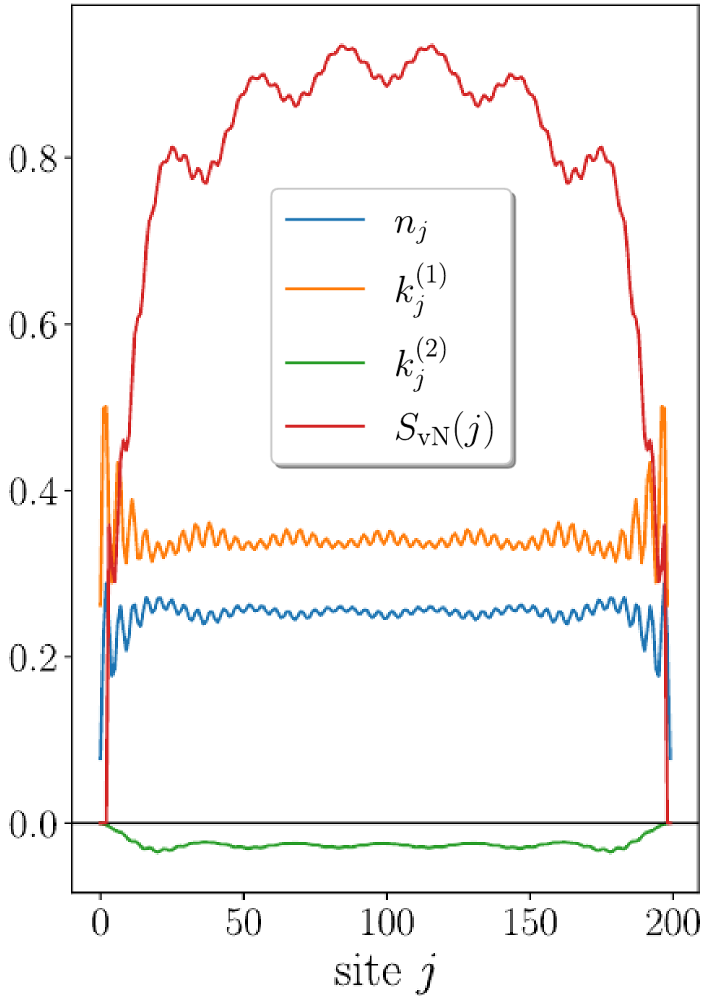


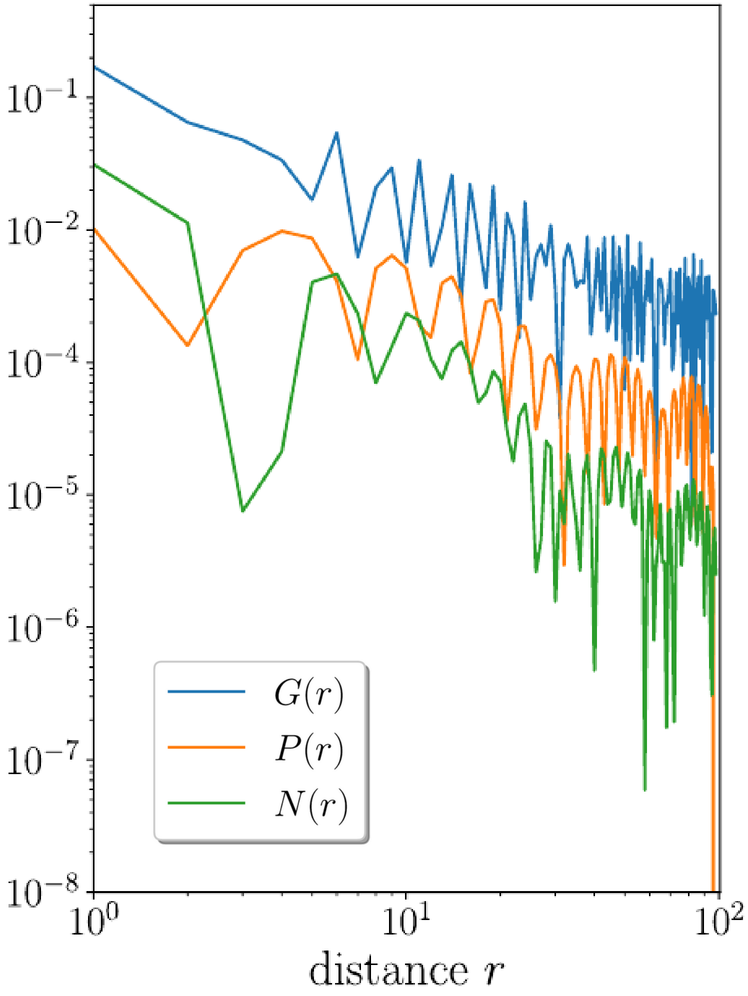
Coexistence phase C



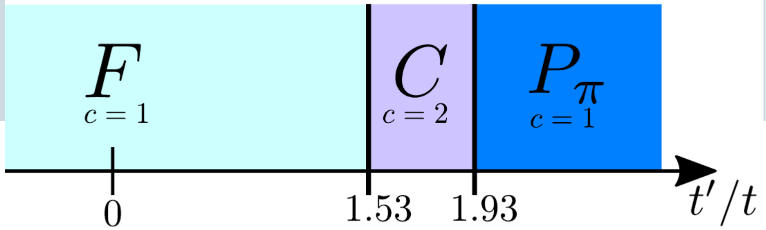
- **What do we observe in the DMRG ?**

two kinds of bumps, for pairs and for unpaired fermions



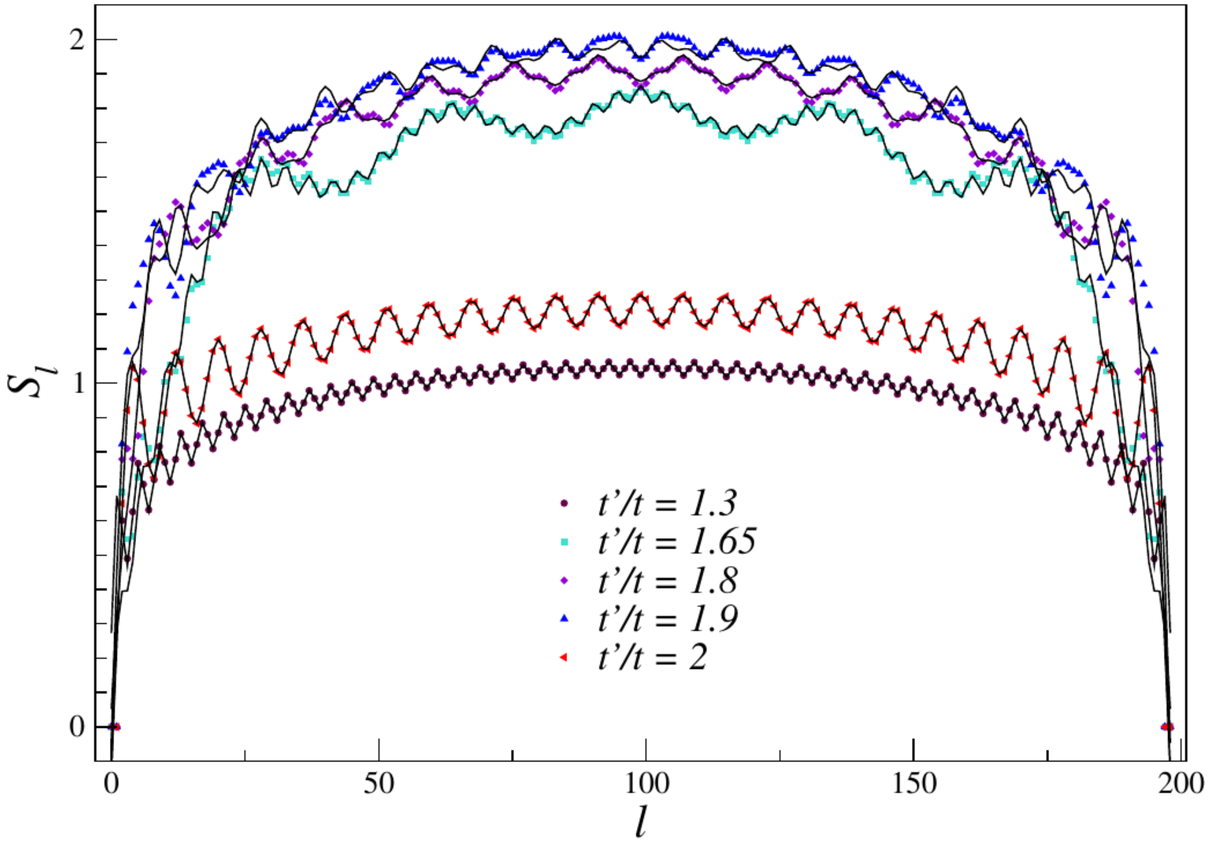


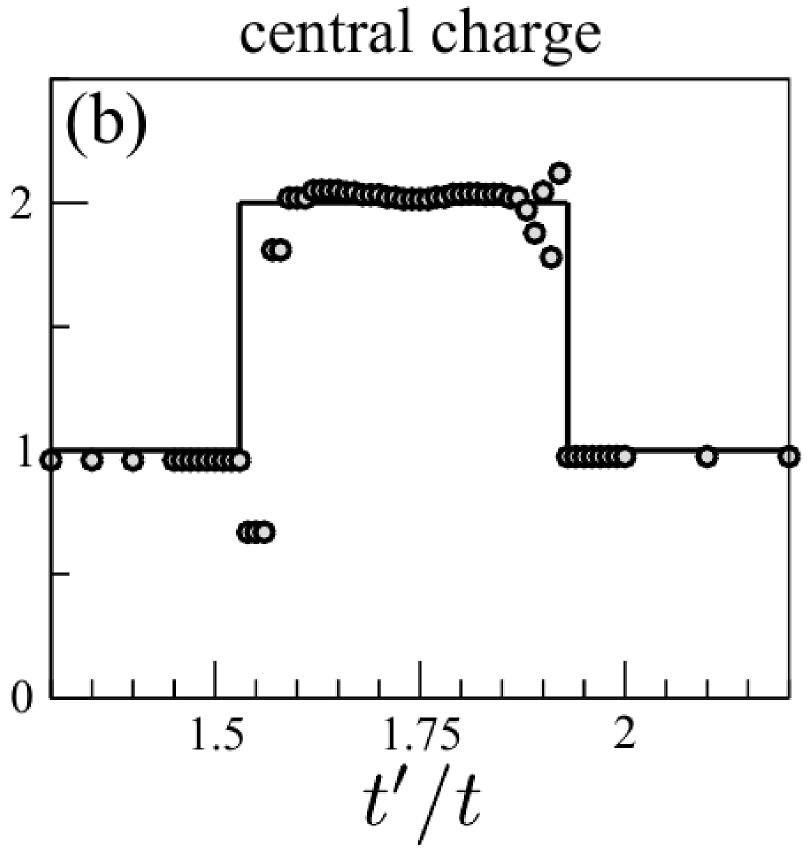
Fitting the entropy



- to get the **central charge**

$$S(\ell) = \frac{c}{6}\log\left[\frac{2L}{\pi}\sin\left(\frac{\pi\ell}{L}\right)\right] + A + C_f\,\langle c^\dagger_{\ell+1}c^\dagger_{\ell} + \text{h.c.}\rangle + C_b\,\langle c^\dagger_{\ell+2}c^\dagger_{\ell+1}c_\ell c_{\ell-1} + \text{h.c.}\rangle$$





Effective two-fluid model

- **Assuming two independent degrees of freedom** : unpaired fermions and bosons (pairs)

$$H_{2F} = H_f + H_b \qquad H_f = -\,t \sum_j d_j^\dagger d_{j+1} + \text{h.c.} \qquad H_b = +\,t' \sum_j \sigma_j^+ \sigma_{j+1}^- + \text{h.c.}$$

parameters : fermions and bosons densities $n_{f,b} = N_{f,b}/L$

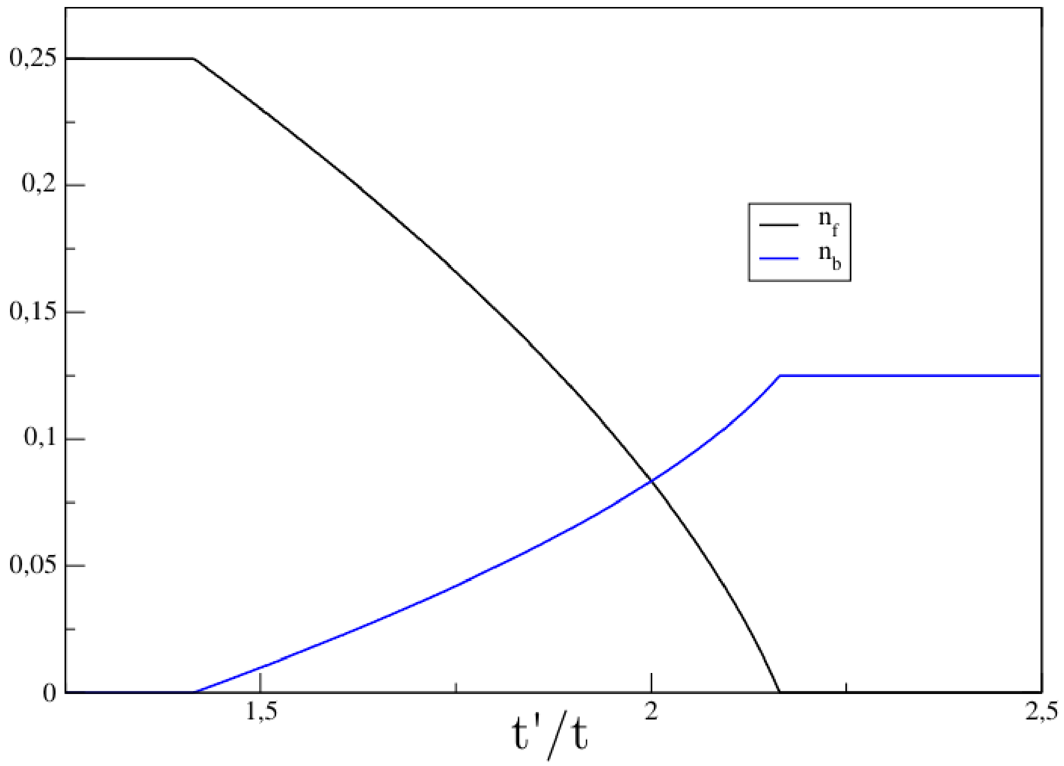
constraint : $n = n_f + 2n_b$

variational energy

$$e_{2F} = -\frac{2t}{\pi}\left[\sin\left(\pi n_f\right) + \tau \sin\left(\pi \frac{n - n_f}{2}\right)\right]$$

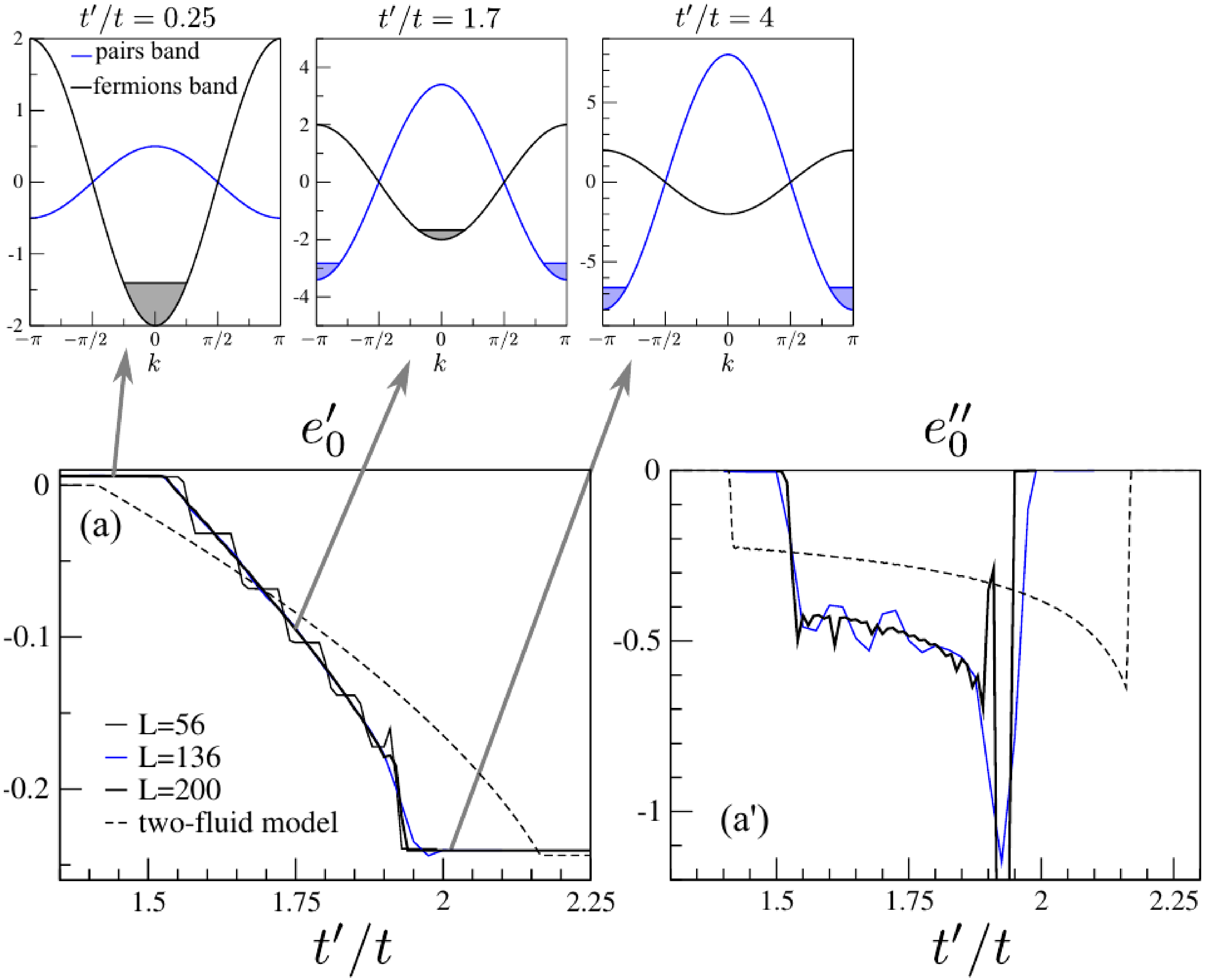
Remark : we use *L* sites for the bosons

=> minimization gives the optimal n_f



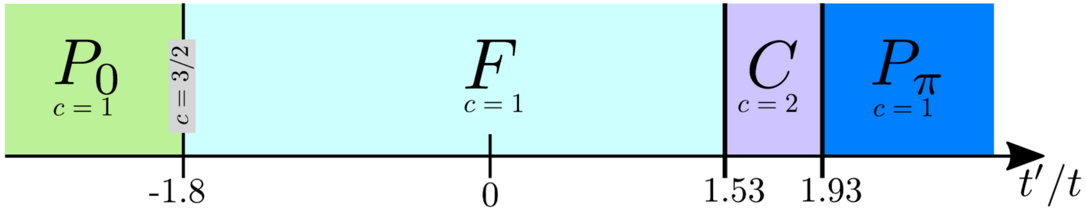
Comparison with numerics

- **Simple band filling picture**
- **Comparison with DMRG**
  ground-state energy e_0
  and its derivatives
- steps are finite-size effects reflecting the add of each pair in the system



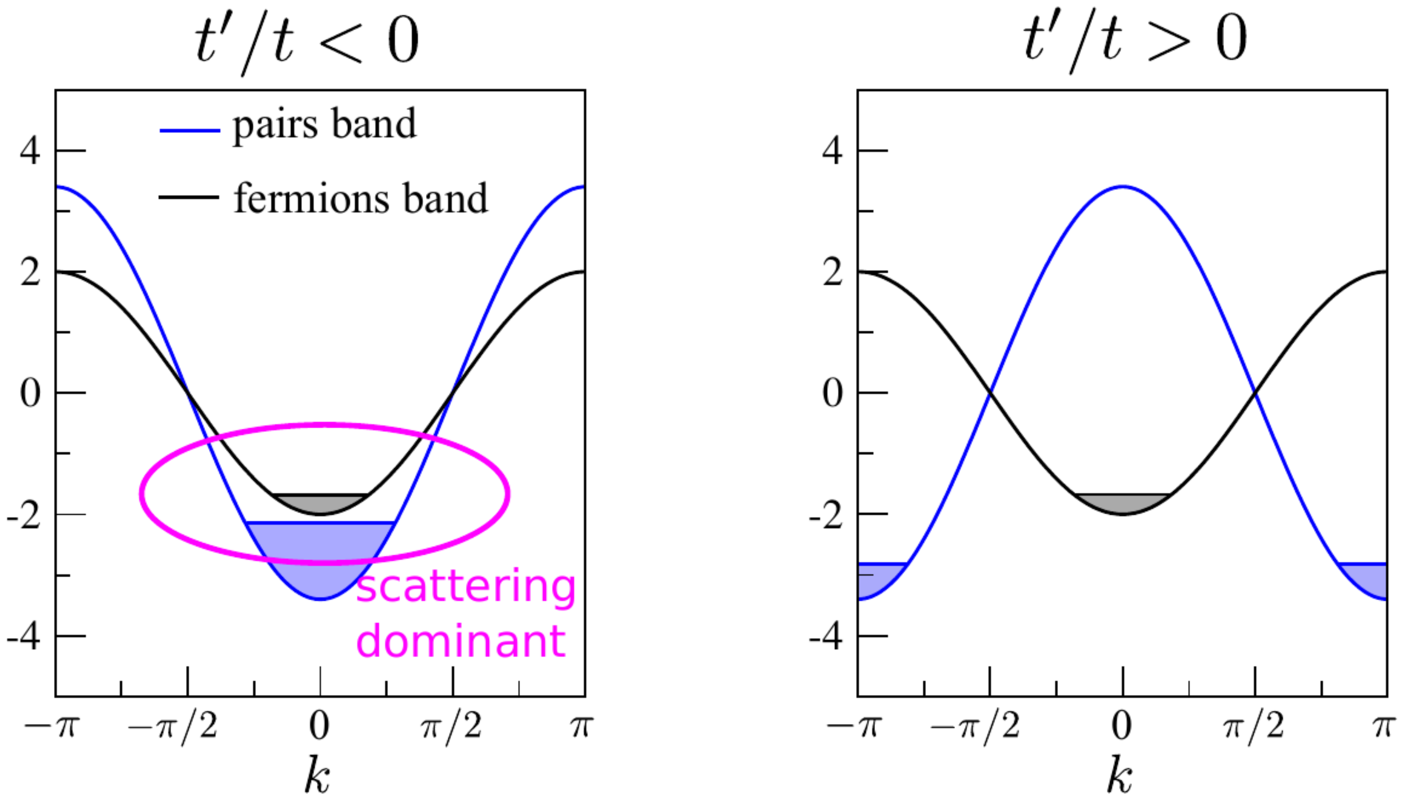
Qualitative consideration

- Why such an asymmetry between *t'* >0 and *t'*<0 ?

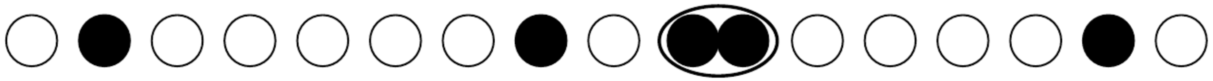


- Why pairs seem to hardly interact with remaining fermions ?

- **A *k*-space argument** : scattering processes should conserve total momentum



Estimates for the critical points



- **DMRG first critical point** $\tau_{c1} \simeq 1.53$

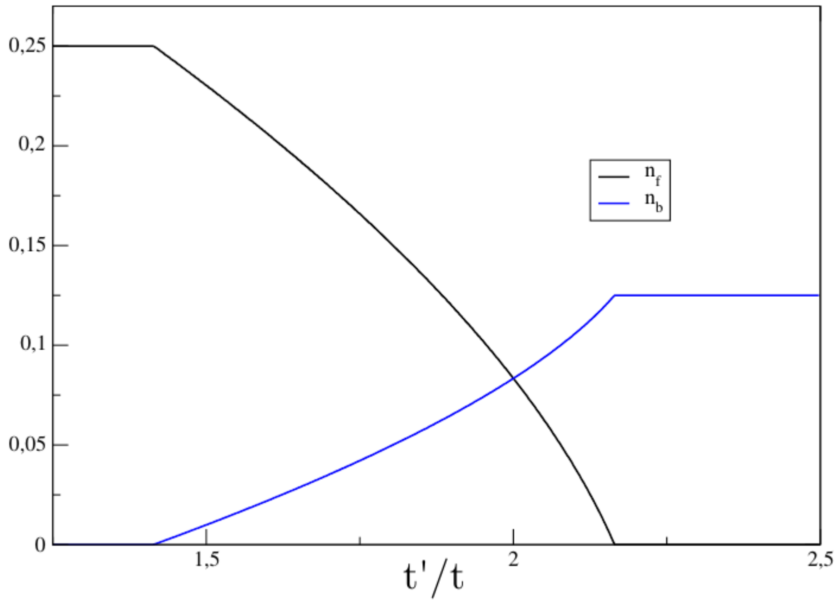
  Bare two-fluid model without interaction

  $$\tau_{c1} = 2\cos(\pi n) \simeq 1.41$$

  Model that includes excluded volume effects :

  fermions have only $L - 2N_b$ sites left

  $$\tau_{c1} = 2(1-n)\cos(\pi n) + \frac{2}{\pi}\sin(\pi n) \simeq 1.51$$



- **DMRG second critical point** $\tau_{c2} \simeq 1.93$

  bare two-fluid model

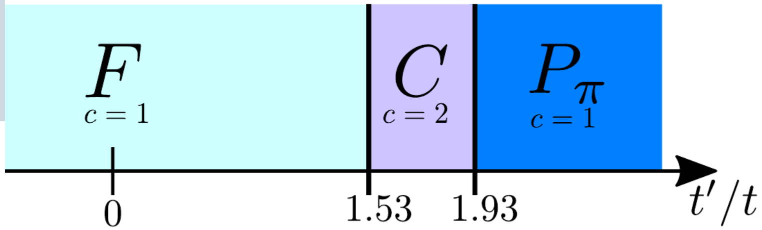
  $$\tau_{c2} = 2/\cos(\pi n/2) \simeq 2.16$$

  caging picture

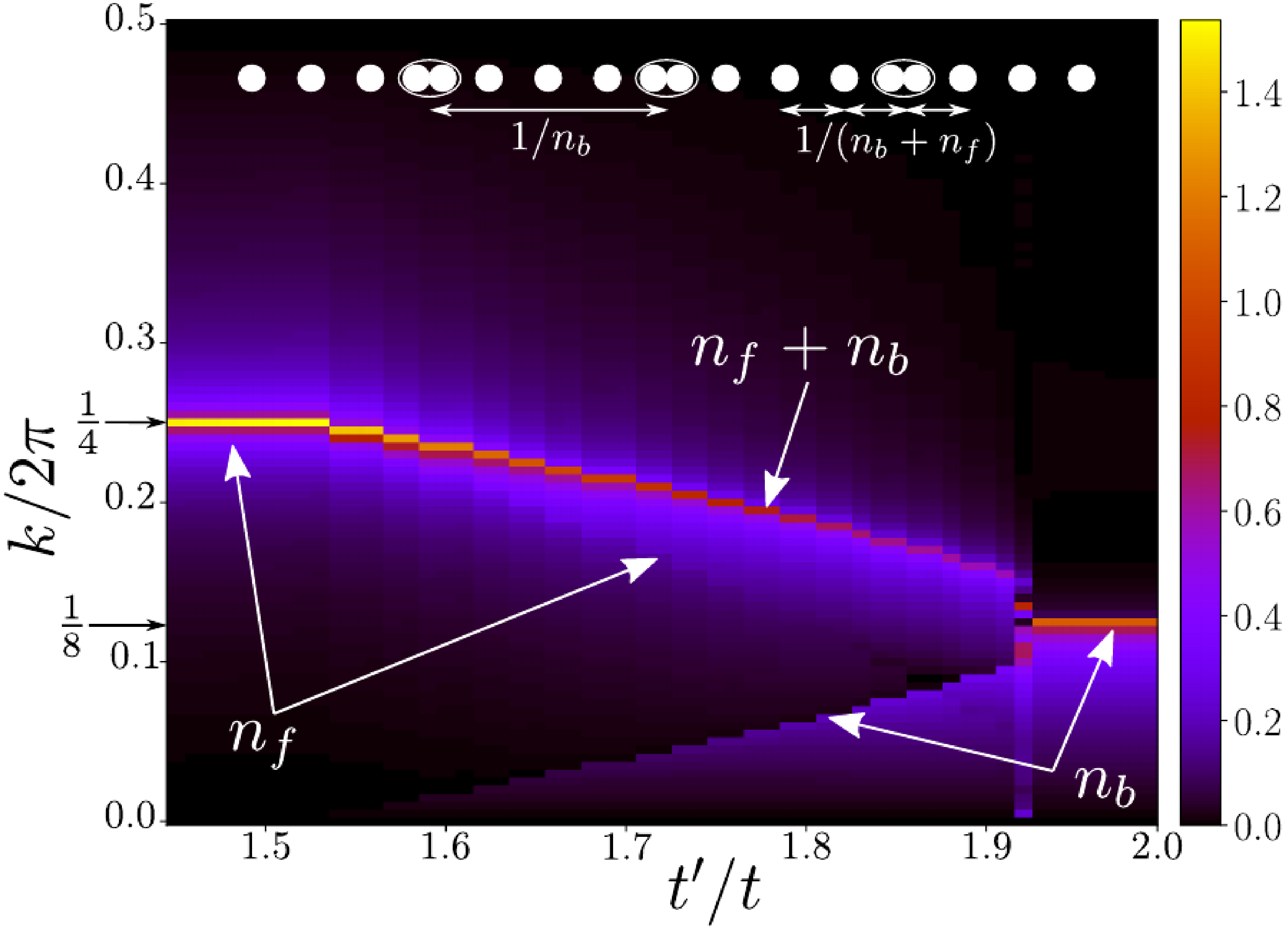
  $$\tau_{c2} = 2$$

Two impurity-like problems !

Probing the intervening C phase



- **Goal** : accessing the evolution of $n_{f,b}$
- **Density like structure factor**
  using open boundary conditions
  $$S(k) = \sum_j e^{-ikj}(\langle \hat{n}_j \rangle - n)$$
  
- **In *F* and *P*$_\pi$ phases**
  Luttinger liquid fluctuations at
  $2k_f = 2\pi n$ and $2k_b = \pi n$
- **In the *C* phase**
  main fluctuations at
  $k = 2\pi(n_f + n_b)$
  secondary peaks at
  $k = 2\pi n_b$
  $k = 2\pi n_f$



Further tests of the two-fluid model

- **Problem** : operators $\hat{c}_j$ and $\hat{c}_j \hat{c}_{j+1}$ capture both unpaired fermions and pairs

- **New operators for fermions and pairs**

$$\hat{f}_j^\dagger = (1 - \hat{n}_{j-1})\hat{c}_j^\dagger (1 - \hat{n}_{j+1}),$$

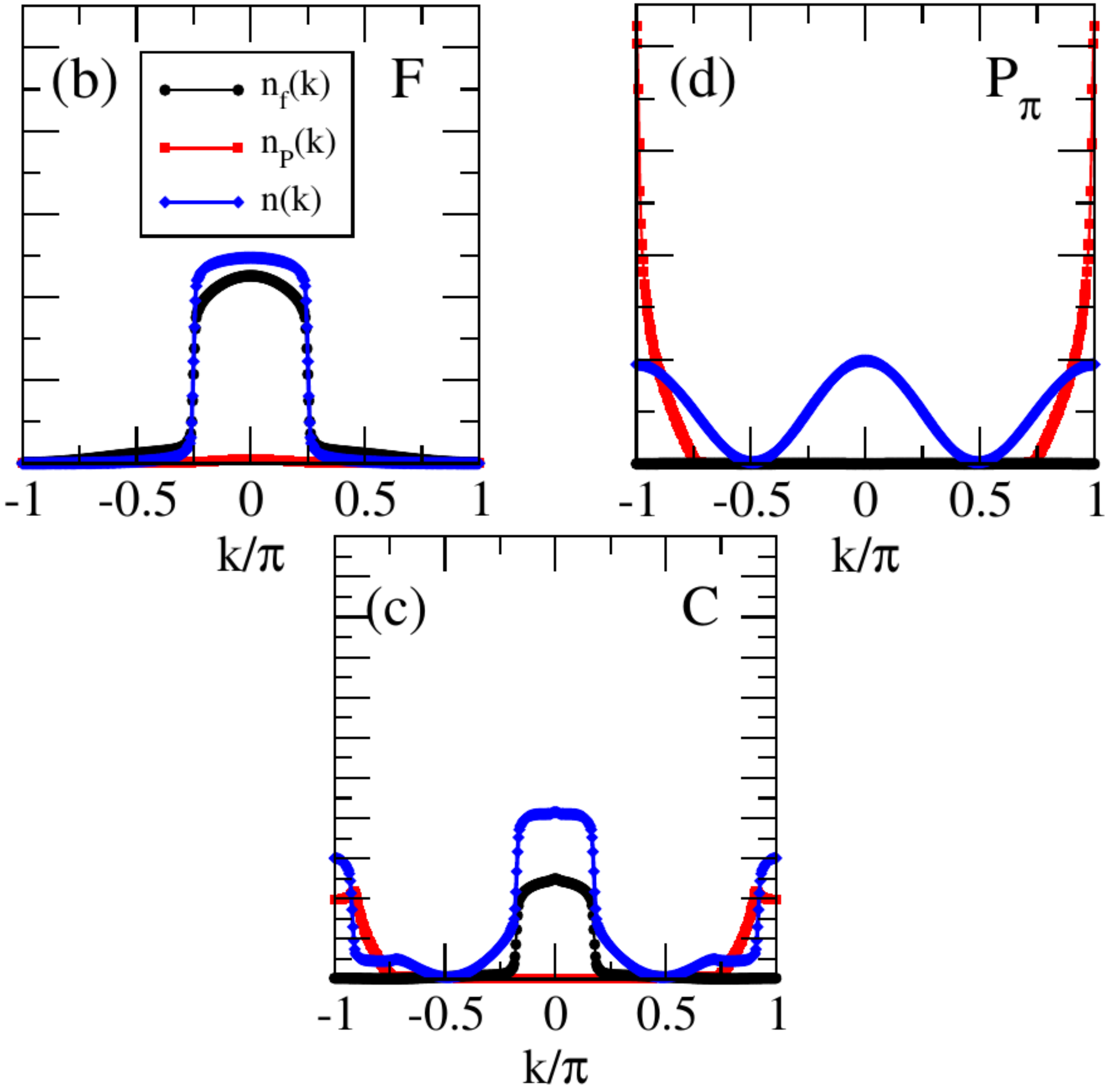
$$\hat{P}_j^\dagger = (1 - \hat{n}_{j-1})\hat{c}_j^\dagger \hat{c}_{j+1}^\dagger (1 - \hat{n}_{j+2}),$$

- **Occupation factors**

$$n(k) = \frac{1}{L} \sum_{j,j'} e^{ik(j-j')} \langle \hat{c}_j^\dagger \hat{c}_{j'} \rangle$$

$$n_f(k) = \frac{1}{L} \sum_{j,l} e^{ik(j-l)} \langle \hat{f}_j^\dagger \hat{f}_l \rangle;$$

$$n_P(k) = \frac{1}{L} \sum_{j,l} e^{ik(j-l)} \langle \hat{P}_j^\dagger \hat{P}_l \rangle.$$

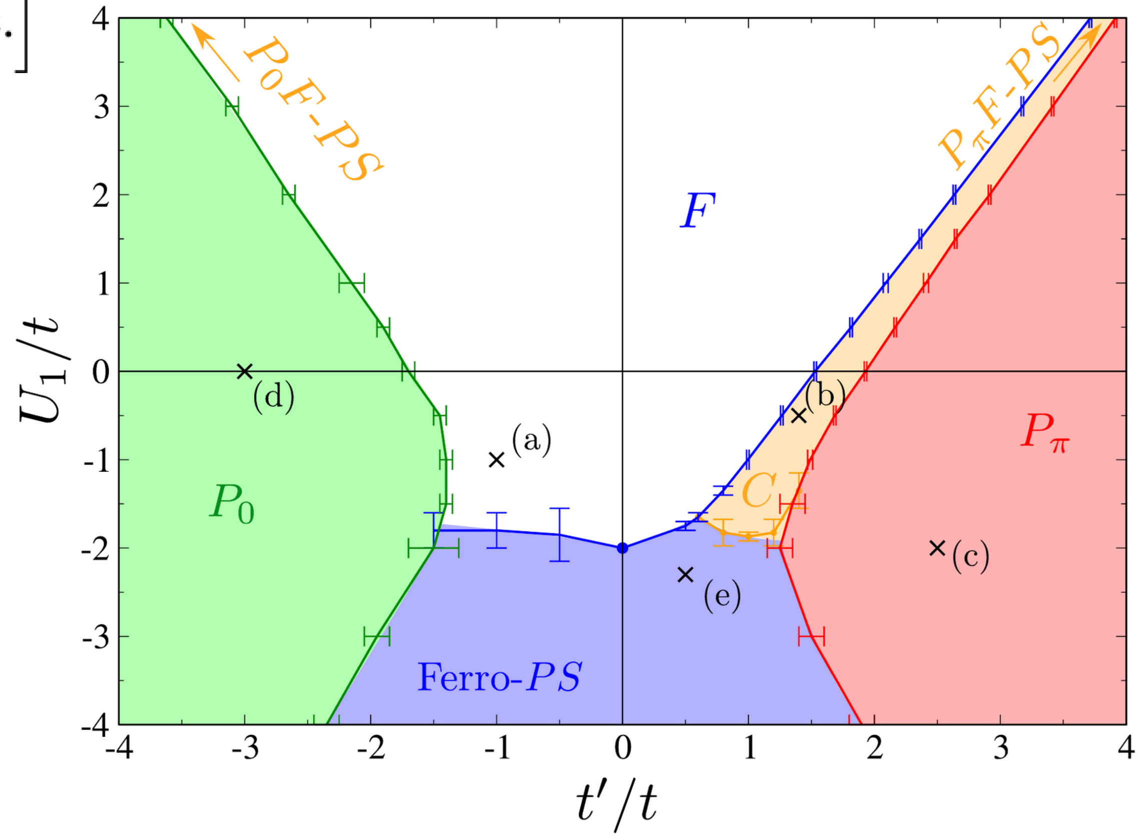


Extensions : interactions, phase separation and trimers formation

Chain of size *L* with spinless fermions with density $n = 0.25$

$$H = -t \sum_j \left[c_j^\dagger c_{j+1} + \text{h.c.} \right] - t' \sum_j \left[c_{j+1}^\dagger c_j^\dagger c_j c_{j-1} + \text{h.c.} \right]$$

$$+ U_1 \sum_j \hat{n}_j \hat{n}_{j+1}$$



Phase diagram

F : regular fermionic Luttinger liquid
P_0 : paired phase with *k* =0 pairs
P_π : paired phase with *k* =π pairs
C : coexistence phase
PS : phase separation phases

Attractive U_1 and the Ferro-PS phase

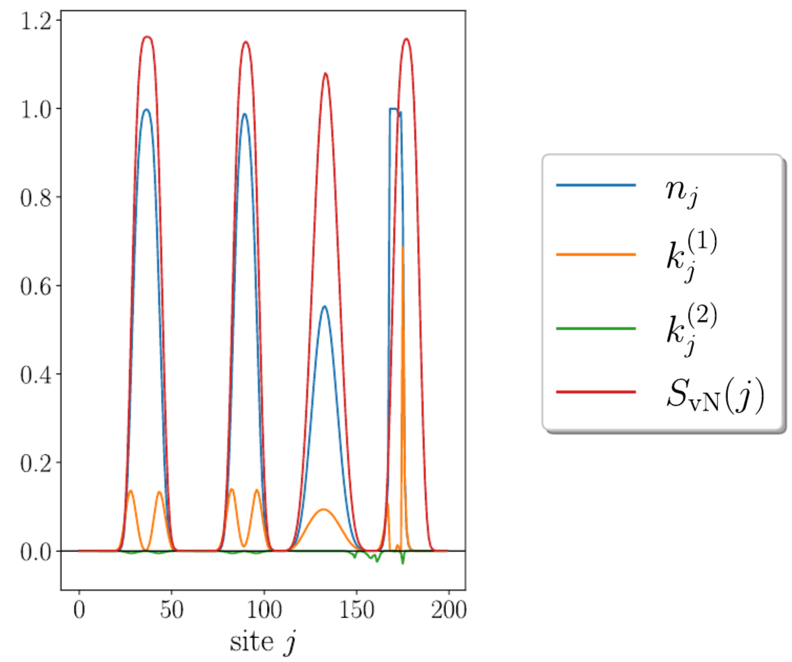
- maps onto the **ferromagnetic phase of the XXZ model**

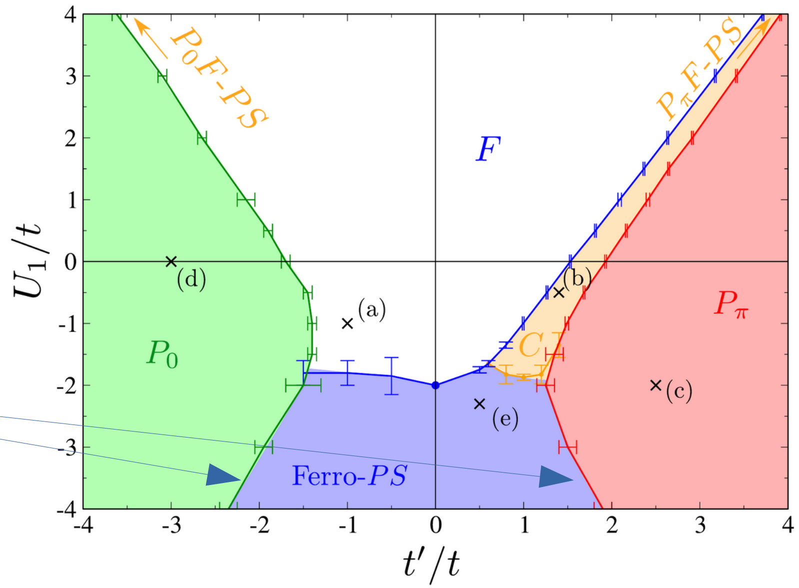
- fermions glue together with negative U_1
  lots of low-energy states with domains

- for t =0, within the subspace of paired states
  the effective Hamiltonian reads

$$\hat{H} = t' \sum_{j=1}^{L_b} \left[\hat{\sigma}_j^+ \hat{\sigma}_{j+1}^- + H.c. \right] + \\ + \frac{U_1}{4} \sum_{j=1}^{L_b} \left(1 + \hat{\sigma}_j^z\right) \left(1 + \hat{\sigma}_{j+1}^z\right)$$

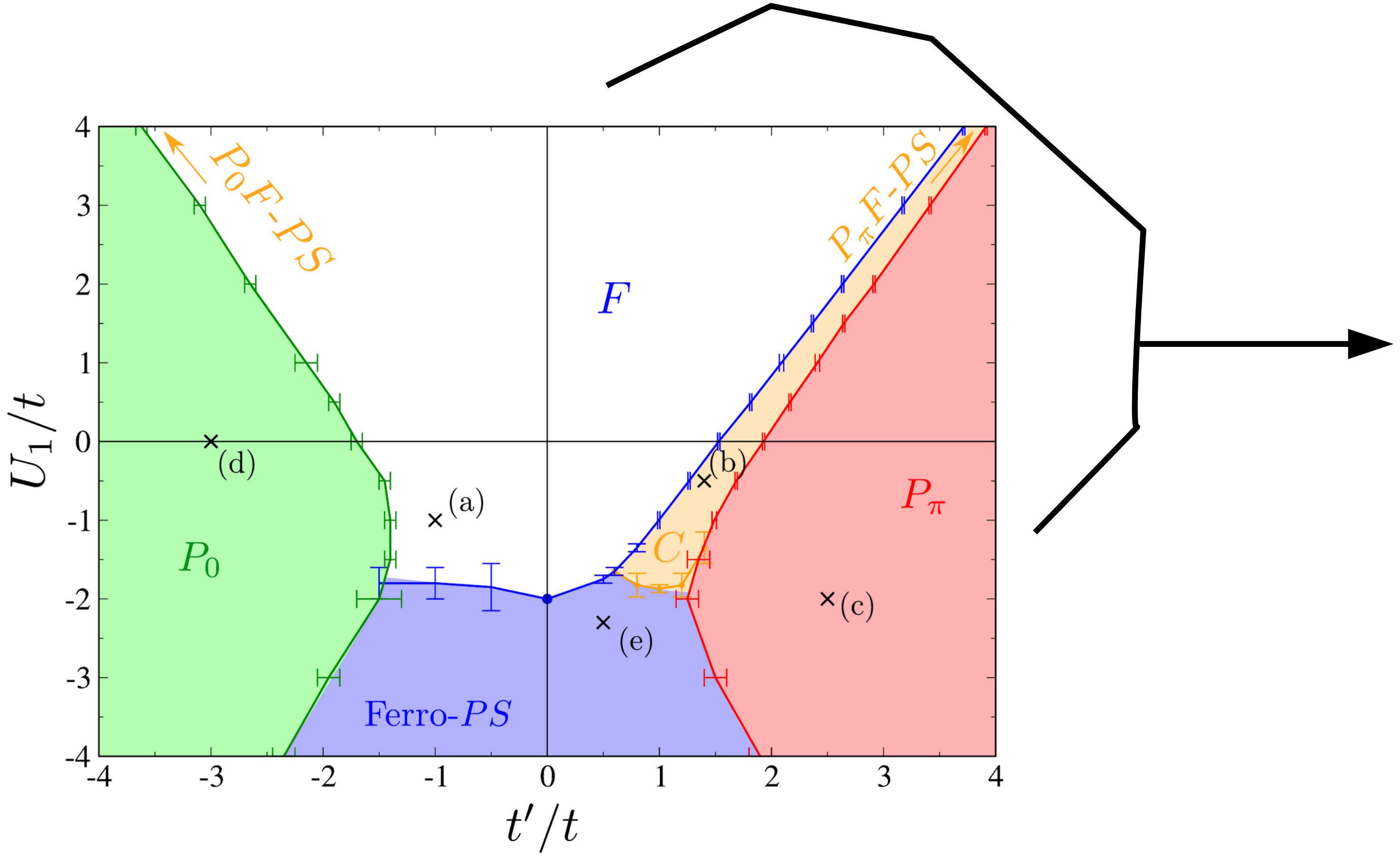
an XXZ model with a transition to the ferromagnetic state at $U_1/t' = -2$ gives the two oblique lines in the phase diagram

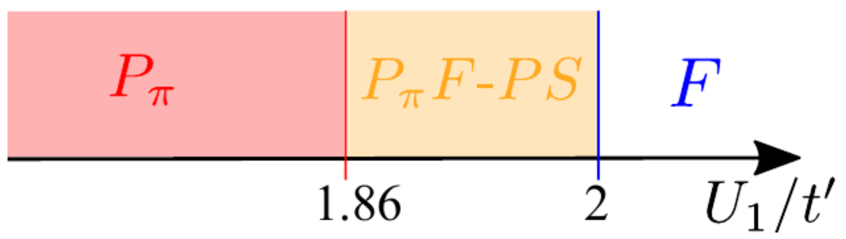




Repulsive U_1 : folding the phase diagram

- Large U_1 and large t' limit



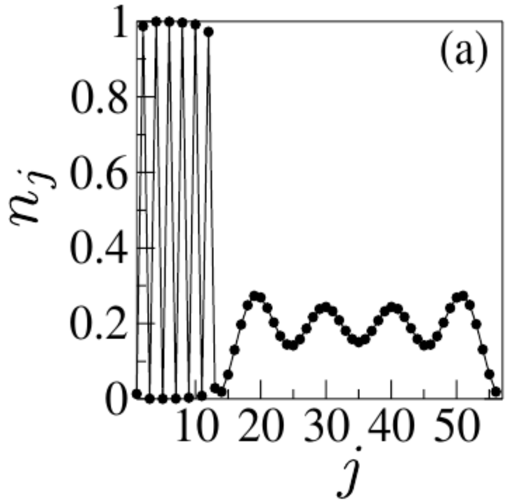


+ study @ $t << t'$

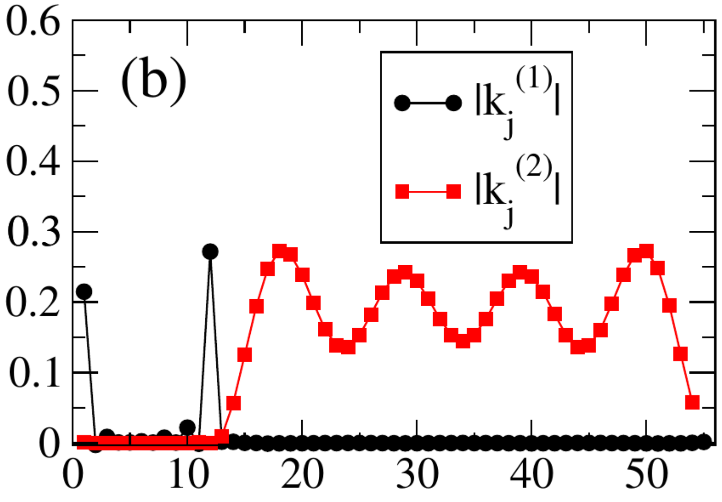
DMRG observations => phase separation !

- **Two typical situations**

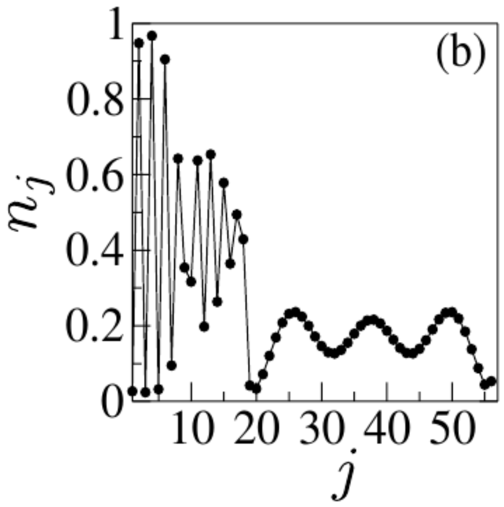
charge-density-wave state of fermions
next to Luttinger liquid of pairs

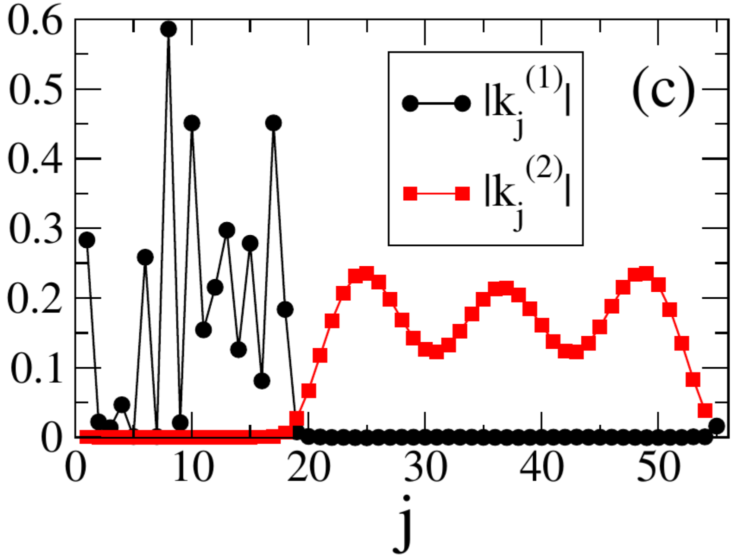


@ t =0



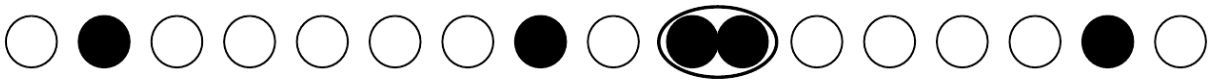
Luttinger liquid of fermions
next to Luttinger liquid of pairs





Repulsive U_1 : simple views on the t =0 limit

- U_1 tends to break pairs into distant fermions



  a single pair has kinetic energy -2t'

  a « Fermi sea » of pairs has energy

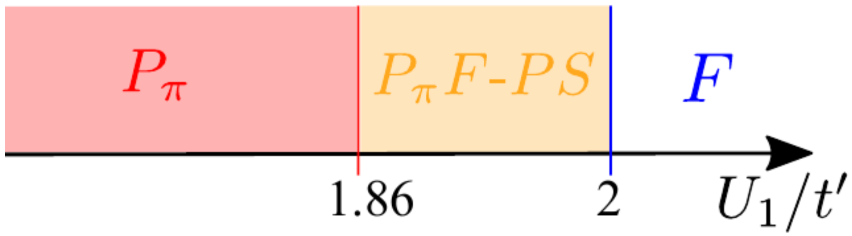
  $-2t' \cos\left(\pi n/(2-n)\right) \sim -1.8t'$

  « isolated » fermions states has zero energy

- **Two consequences**

  => for $U_1/t' > 2$, the *F* phase is favored

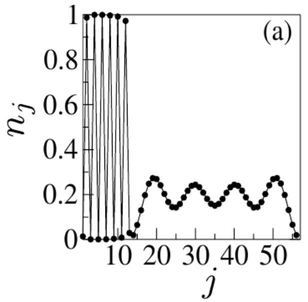
  => for $U_1/t' \lesssim 1.8$, the paired phase is favored



What is in between ???

Phenomenological model for t =0

- Same idea as for van der Waals fluid => look for a **two domains solution**
- **Ansatz for the energy of the CDW phase separated state**



N_f unpaired fermions in a CDW state over $2N_f$ sites

$\frac{N-N_f}{2}$ pairs over the remaining $L-2N_f$ sites to reach only $L-2N_f-\frac{N-N_f}{2}$ sites contribute to the kinetic energy

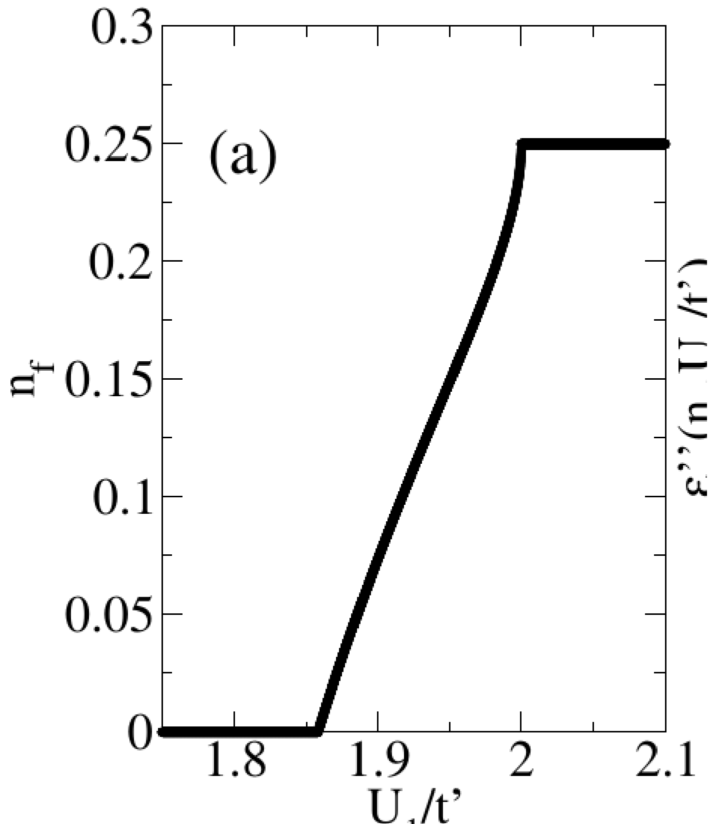
U_1 merely acts as a chemical potential for pairs

Energy parametrized by $n_f = N_f/L$ and $U_1/t' = \tan\theta$

$$\mathcal{E}(n_f,\theta) = -\frac{2}{\pi}\left(1-2n_f-\frac{n-n_f}{2}\right)\sin\left[\pi\frac{n-n_f}{2\left(1-2n_f-\frac{n-n_f}{2}\right)}\right] + \frac{n-n_f}{2}\tan\theta$$

- **First critical point prediction**

$$\left(\frac{U_1}{t'}\right)_{c1} = \frac{6}{\pi}\sin\left(\frac{\pi n}{2-n}\right) - \frac{4(2n-1)}{2-n}\cos\left(\frac{\pi n}{2-n}\right) \approx 1.858$$



Extending the phenomenology to $t \neq 0$

- Still a two domains solution but with the possibility of a **liquid for unpaired fermions** in which neighbouring fermions are forbiden because of large U_1

  occupies a fraction of the total size $l_f = L_f/L$ and has density n_f

  with constraints : $n_f \in [0,n]$ and $l_f \in [2n_f, n_f+1-n]$

  if n_f =0.5, this includes the CDW state

- **Variational energy** : $\tan\theta = U_1/t'$ and $r = \sqrt{\left(\frac{U_1}{t}\right)^2 + \left(\frac{t'}{t}\right)^2}$

$$\mathcal{E}_2(n_f, l_f, r, \theta) = \begin{cases} -\frac{\cos\theta}{\pi}(2-n)\sin\left(\frac{\pi n}{2-n}\right) + \sin\theta\frac{n}{2}, & \text{if } (n_f, l_f) = (0,0) \\ -\frac{2}{\pi r}(1-n)\sin\left(\frac{\pi n}{1-n}\right), & \text{if } (n_f, l_f) = (n,1) \\ -\frac{2}{\pi r}(l_f - n_f)\sin\left(\frac{\pi n_f}{l_f - n_f}\right) - \frac{\cos\theta}{\pi}\left[2(1-l_f) - n + n_f\right]\sin\left[\frac{\pi(n-n_f)}{2(1-l_f)-n+n_f}\right] + \sin\theta\frac{n-n_f}{2} \end{cases}$$

pairs only

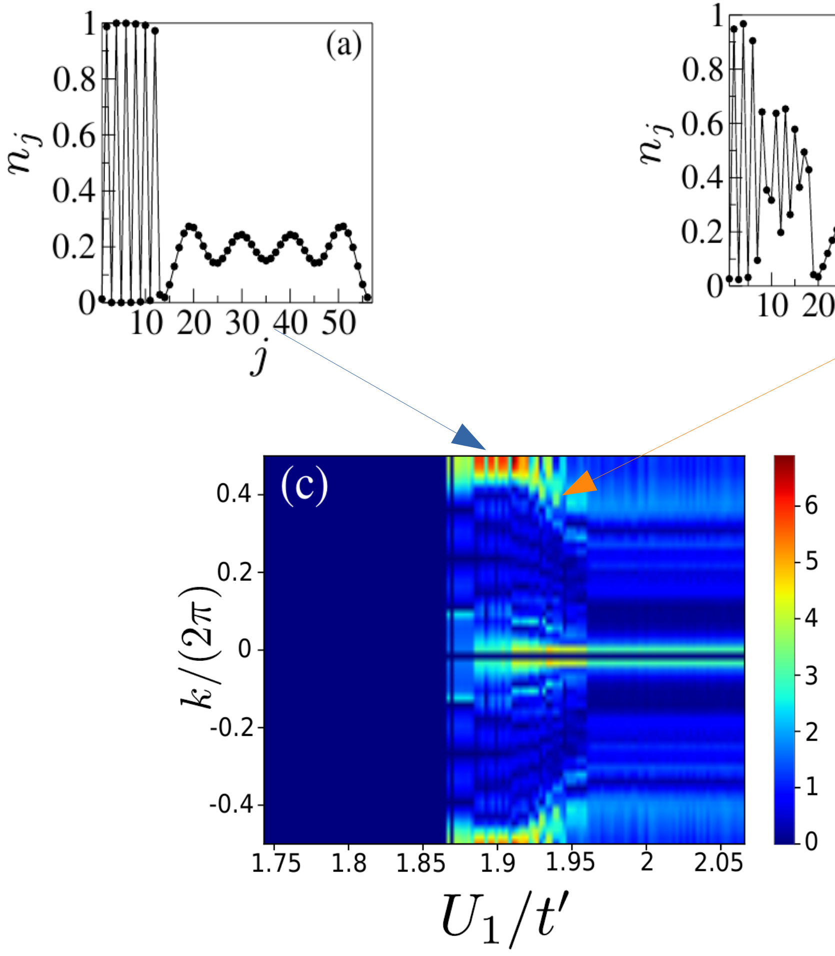
fermions only

two domains solution (phase separation)

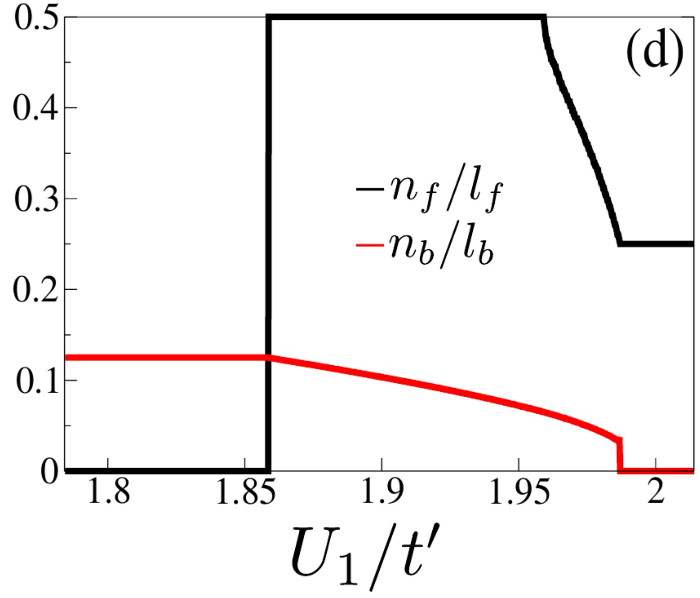
Comparing with DMRG

- using periodic boundary conditions and a small *t*, difficult simulations

DMRG

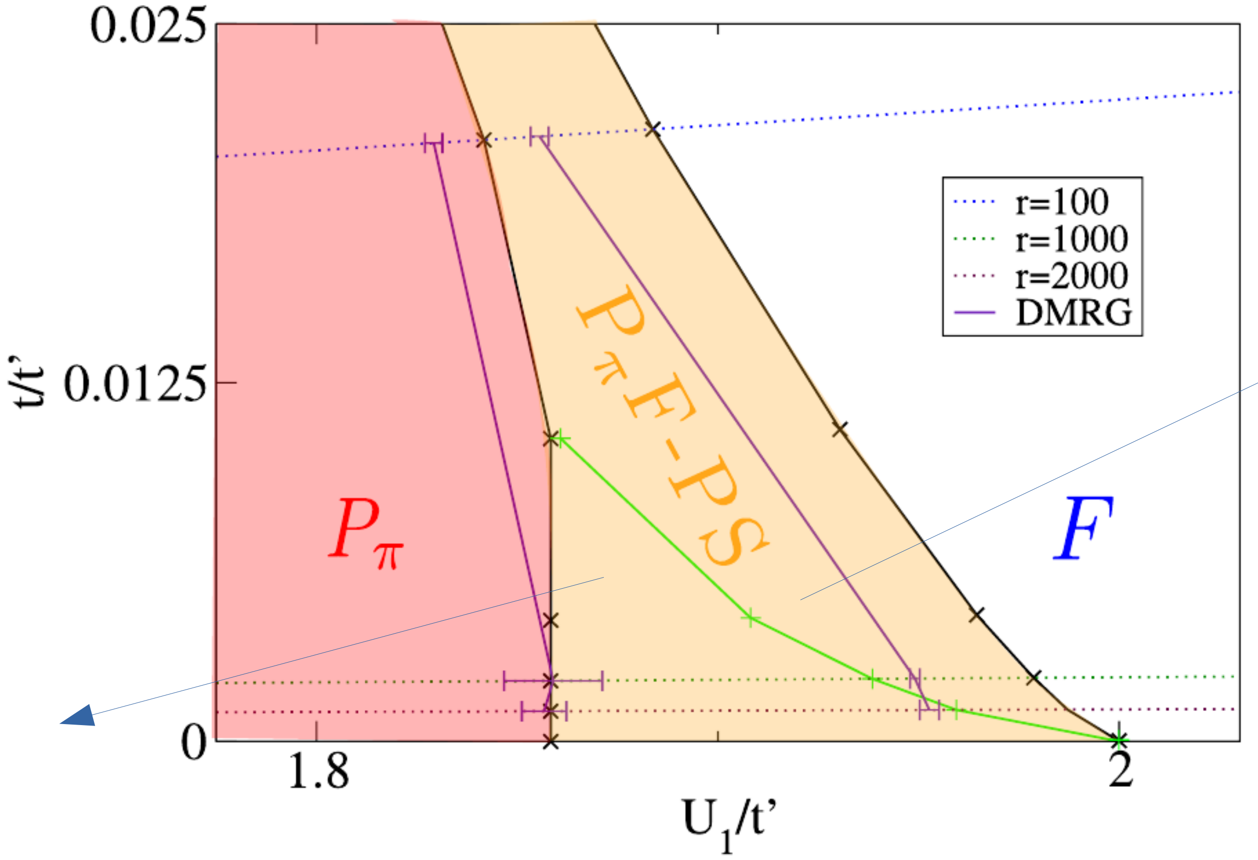


Effective model



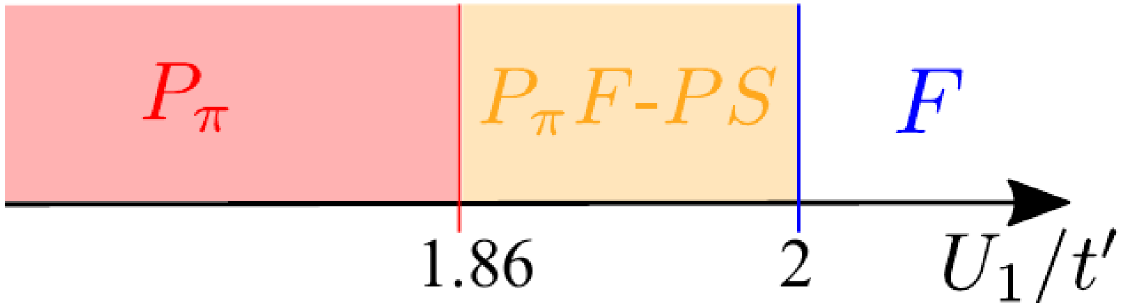
Phase diagram in the *t* << *t'* limit

- collecting results



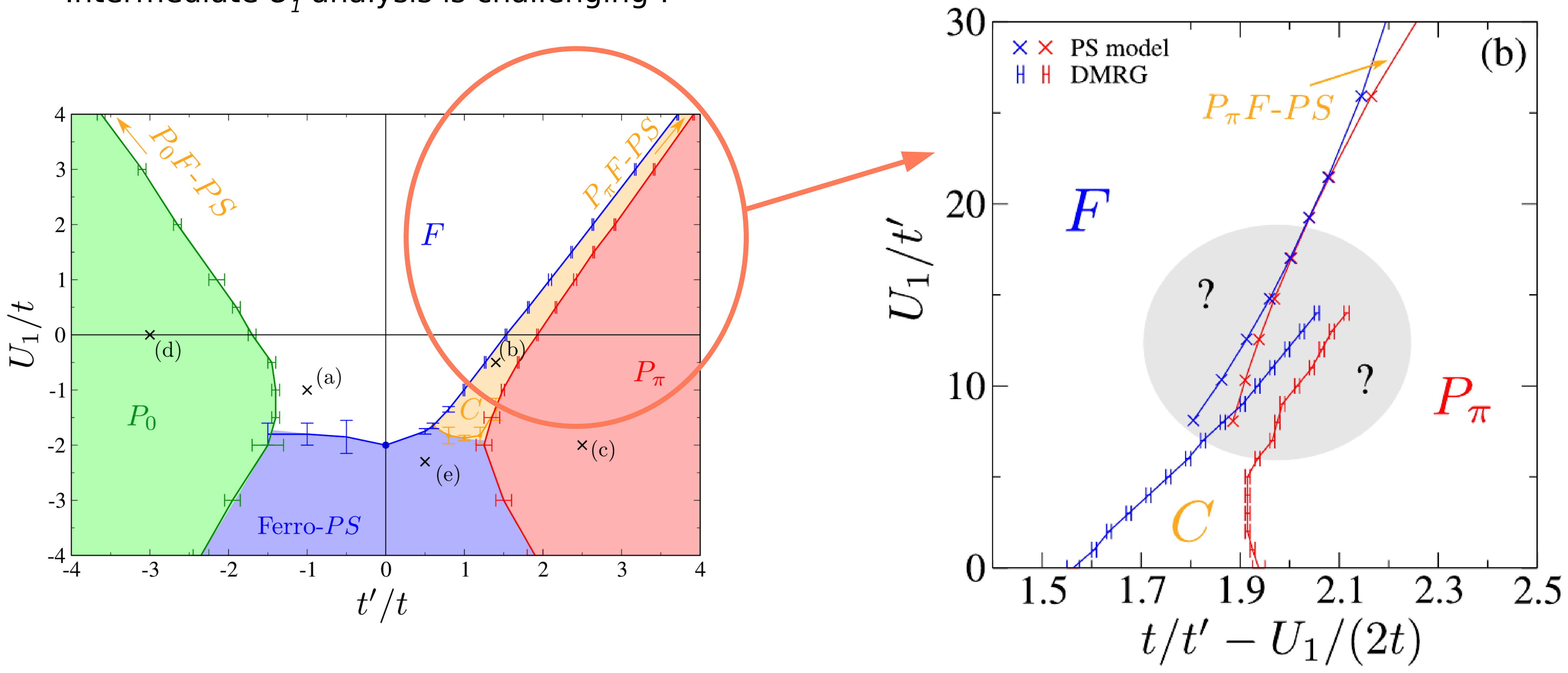
with a fermionic liquid domain

with a CDW domain



Trying to connect to the original diagram

- collecting results, **how do we go from coexistence to phase separation ?** Intermediate U_1 analysis is challenging !



Conclusion

Still exist surprises in 1D physics !

- a rich phase diagram for a simple model
- remarkable emergent two-fluid picture and phase coexistence / separation
- importance of DMRG as a guide and succes of phenomenology
- challenges for field theory

Perspectives

- Preliminary results on trimer formation and coexistence with similar model !
- Increasing density should increase effective interactions between pairs and fermions
- Higher dimension ?

Thanks a lot for your attention !