Kinetic formation of trimers in a spinless fermionic chain

L. Gotta[1], L. Mazza[1], P. Simon[2], G. Roux[1]

[1] *Laboratoire de Physique Théorique et Modèles Statistiques, CNRS, Université Paris-Saclay, France*

[2] *Laboratoire de Physique des Solides, CNRS, Université Paris-Saclay, France*

Model and main result

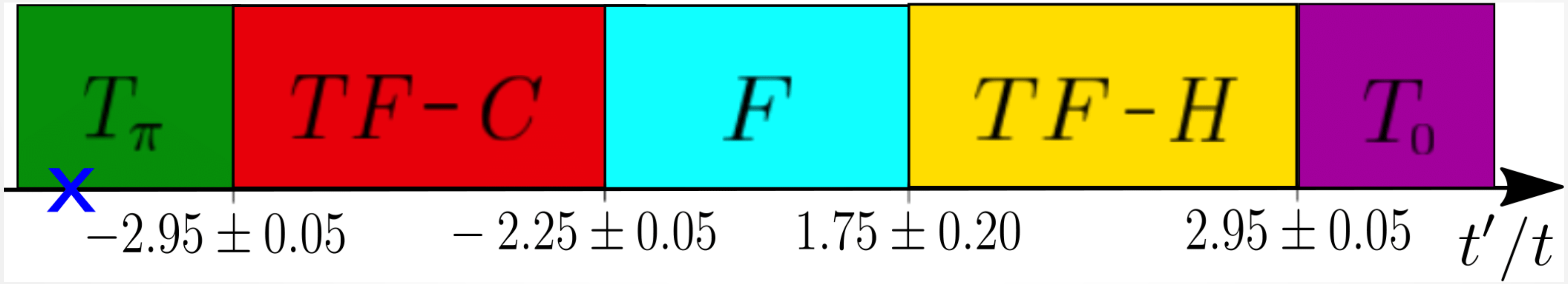
Hamiltonian (spinless fermions on a 1D lattice, $n = \frac{1}{4}$ filling)

$$\hat{H} = -t \sum_j \left(\hat{c}_j^\dagger \hat{c}_{j+1} + H.c. \right) - t' \sum_j \left(\hat{T}_j^\dagger \hat{T}_{j+1} + H.c. \right)$$

with trimer annihilation operator $\hat{T}_j = \hat{c}_j \hat{c}_{j+1} \hat{c}_{j+2}$

Result

→ zero temperature phase diagram of the model:



- $T_{0,\pi}$ phases: Luttinger liquid phases with molecular granularity
- F phase: weak coupling Luttinger liquid phase
- $TF-C, H$ phases: coexistence of unbound fermions and trimers

F and $T_{0,\pi}$ phases

1) F phase: $t' \to 0$ ➡ $\hat{H} \to \hat{H}_F = -t\sum_j \hat{c}_j^\dagger \hat{c}_{j+1} + H.c.$

→ standard Luttinger liquid theory holds

2) $T_{0,\pi}$ phase: $t \to 0$ ➡ $\hat{H} \to \hat{H}_T = -t'\sum_j \hat{T}_j^\dagger \hat{T}_{j+1} + H.c.$

→ search for $|\psi_{GS}\rangle$ in the subspace $\mathcal{H}_M$

of fully molecular fermionic configurations:

map to effective fermionic chain

map to effective free-fermion Hamiltonian

$|\bullet\bullet\bullet\rangle \to |1\rangle$

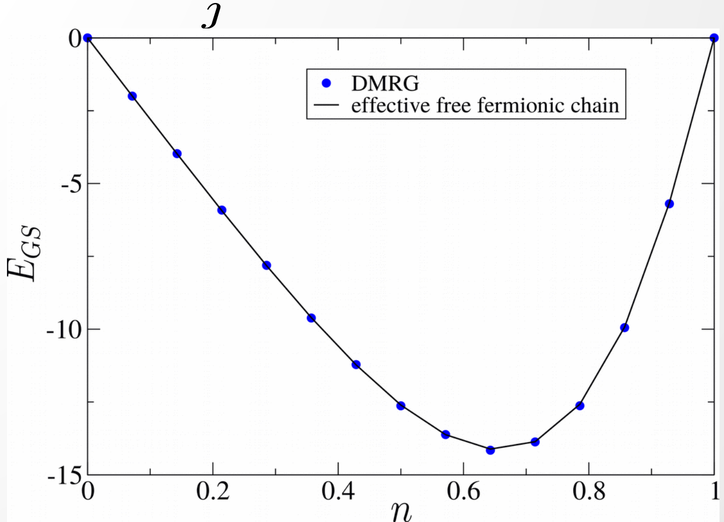
$|\circ\rangle \to |0\rangle$

$$\hat{H}_T \equiv -t'\sum_j{}' \hat{f}_j^\dagger \hat{f}_{j+1} + H.c.$$

Dispersion relation: $\epsilon_T(k) = -2t'\cos(k)$

→ minimum at $k = 0$ for $t' > 0$ (T_0 phase)

→ minimum at $k = \pi$ for $t' < 0$ (T_π phase)



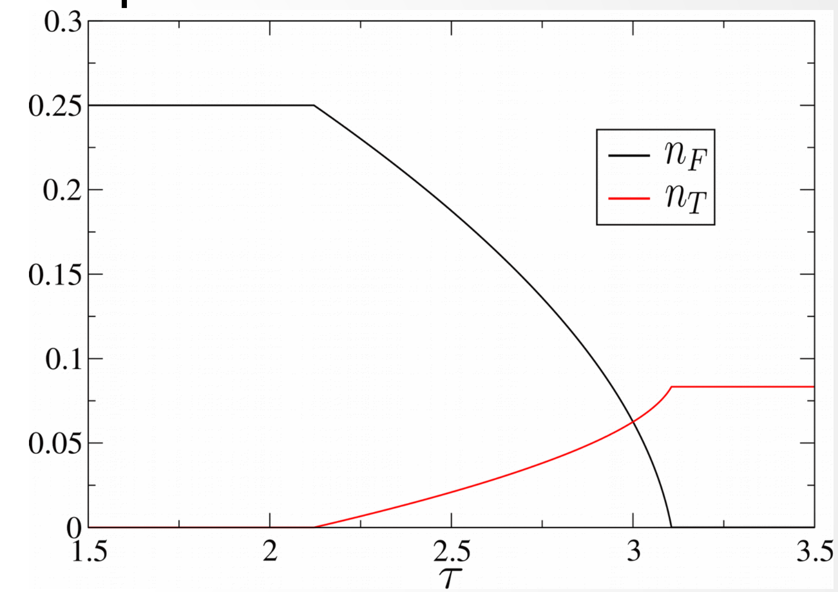
Intermediate phase between F and T_π : the $TF-C$ phase

Momentum mismatch → non-interacting two-fluid description

- assume system to be populated by two species of particles:

$$\hat{H}_{2F} = -t \sum_j \hat{f}_j^\dagger \hat{f}_{j+1} - t' \sum_j \hat{t}_j^\dagger \hat{t}_{j+1} + H.c.$$

uncoupled fermions   trimers



- minimize total energy density

under the density constraint $n_F + 3n_T = n$

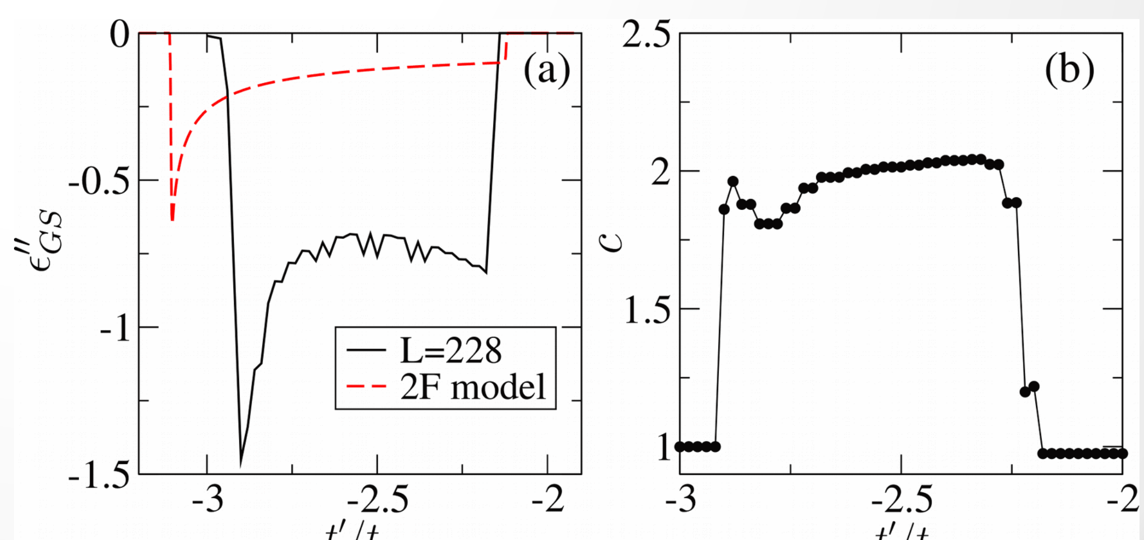
Comparison with DMRG data

- central charge

→ extended region with

2 gapless modes

- energy density criticality



Intermediate phase between F and T_0: the $TF-H$ phase

- Absence of momentum mismatch → add interspecies interactions:

$$\hat{H}_{2F} = -t\sum_j \hat{f}_j^\dagger \hat{f}_{j+1} - t'\sum_j \hat{t}_j^\dagger \hat{t}_{j+1} + g\sum_j \hat{t}_j^\dagger \hat{f}_{j-1}\hat{f}_j\hat{f}_{j+1} + H.c.$$

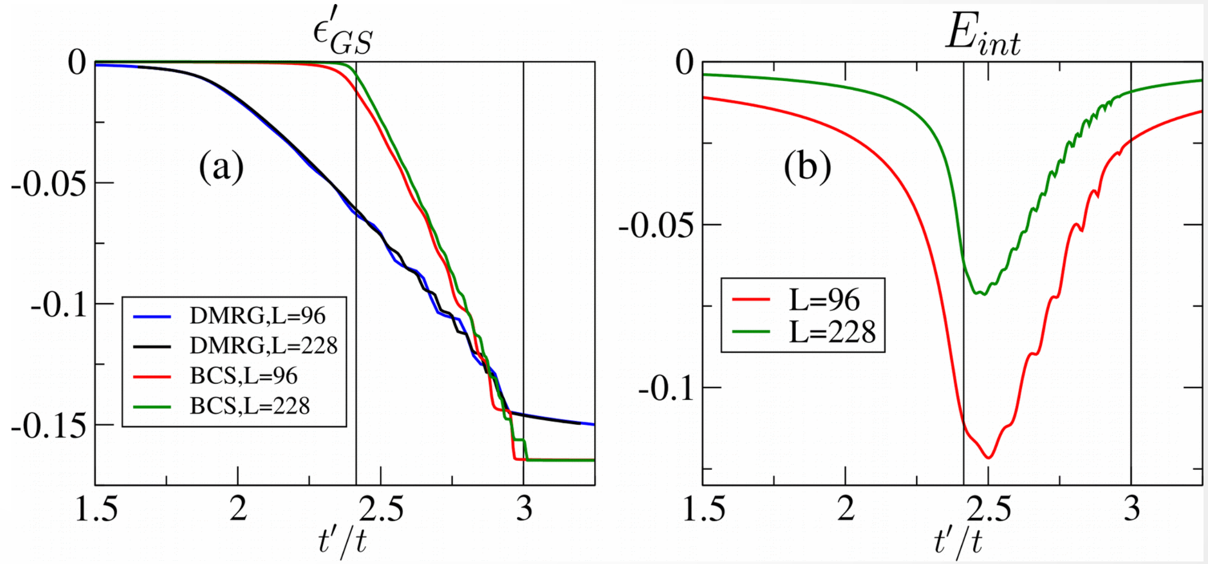
- Introduce variational Ansatz:

$$|\Psi_3\rangle = \prod_{-\frac{k_F}{3}<k<\frac{k_F}{3}} \left(\alpha_k + \beta_k \hat{t}_k^\dagger \hat{f}_{-k_F+\delta_k}\hat{f}_k\hat{f}_{k_F-\delta_k}\right)|n_F\rangle \otimes |v_T\rangle,\ \delta_k \sim 2|k|$$

Finite-size features

→ smooth behavior close to first boundary: strong hybridization

→ sharp second boundary



Thermodynamic limit

→ robustness of finite-size effects both in DMRG data and in variational prediction

→ guess from variational Ansatz: - vanishing of hybridization contribution

- recovery of $t' < 0$ critical behavior

Perspectives on larger multimers

1) Heuristic guess: $\hat{H}_d(t,t') = -t\sum_j \hat{c}_j^\dagger \hat{c}_{j+1} - t'\sum_j \hat{c}_j^\dagger \left(\prod_{l=1}^{d-1} \hat{n}_{j+l}\right) \hat{c}_{j+d} + H.c.$

→ single-particle hopping + hopping term for molecule of size d

- $\hat{c}_j \to e^{i\frac{\pi}{d}j}\hat{c}_j$ ⟹ $\hat{H}_d(t,t') \to \hat{H}_d(e^{i\frac{\pi}{d}}t, -t')$ $\xrightarrow{d \gg 1}$ $\hat{H}_d(t,t') \approx \hat{H}_d(t,-t')$

(emergent symmetry)

2) Energetic signatures on the model with $d=4$:

$$\hat{H} = \sum_j \left(-t\hat{c}_j^\dagger \hat{c}_{j+1} + t'\hat{M}_j^\dagger \hat{M}_{j+1} + H.c.\right) = L(-t\hat{K}_1 + t'\hat{K}_4)$$

with $\hat{M}_j = \hat{c}_j \hat{c}_{j+1} \hat{c}_{j+2} \hat{c}_{j+3}$

→ quantitative agreement between $t' > 0$ and $t' < 0$

→ compare data with two-fluid picture