Bose-Fermi solid and its quantum melting in a one-dimensional optical lattice

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Motivation:

- Tremendous experimental efforts in realizing ultracold ensembles of polar molecules
  - quantum simulation of extended Hubbard models
  - quantum information processing
  - controlled chemistry
  - precision measurements
- Theoretical studies on bosonic or fermionic polar molecules / dipolar atoms
  - Wigner crystallization
  - transition between dipolar superfluid and crystal
- Theoretical studies on Bose-Fermi mixtures in "conventional" ultracold atom systems
  - effect of fermions on the coherence of bosons
  - gapped ''Neel'' state with true long-range order

How about Bose-Fermi mixtures of dipolar particles?

Model and method:

Extended Bose-Fermi Hubbard model in 1D, Neglecting interactions beyond nearest neighbors (NN):

$$H = H_B + H_F + H_{BF},$$

with

$$H_B = -J_B \sum_{\langle i,j\rangle} b_i^\dagger b_j + \frac{U_{BB}}{2}\sum_i n_i^B(n_i^B - 1) + \frac{V_{BB}}{2}\sum_{\langle i,j\rangle} n_i^B n_j^B - \mu_B \sum_i n_i^B,$$

$$H_F = -J_F \sum_{\langle i,j\rangle} f_i^\dagger f_j + \frac{V_{FF}}{2}\sum_{\langle i,j\rangle} n_i^F n_j^F - \mu_F \sum_i n_i^F,$$

$$H_{BF} = U_{BF}\sum_i n_i^B n_i^F + V_{BF}\sum_{\langle i,j\rangle} n_i^B n_j^F$$

In our work, we consider *repulsive interactions*. We assume:

$U_{BB} = U_{BF} = U$ (unit for energy) and $J_B = J_F = J$

Numerical method:

infinite lattice version of the Time-Evolving-Block-Decimation algorithm (iTEBD)

- closely related to DMRG
- developed from the perspective of quantum information
- efficient in simulation of ground state and dynamical properties of 1D quantum lattice models.

Classical limit at J=0:

By comparing with the energies of various configurations at J=0, such as half-filled Bose or Fermi DW and Bose Mott (n=1), it is straight-forward to get the necessary conditions for the existence of stable half-filled Bose-Fermi Solid phase:

$$\mu_B, \mu_F > 2V_{BF}$$

$$2(V_{FF} - V_{BF}) > \mu_F - \mu_B > 2(V_{BF} - V_{BB})$$

Numerical Results:

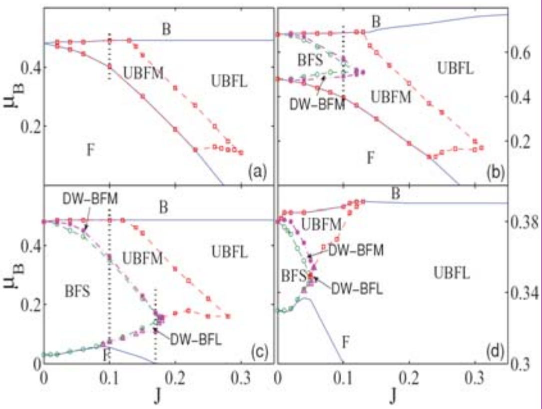

Fig. 1 Ground state phase diagram of the extended Bose-Fermi Hubbard model at fixed fermion chemical potential. (a) no NN interaction; (b) boson-boson NN interaction only; (c) fermion-fermion NN interaction only; (d) boson-boson, fermion-fermion, and boson-fermion NN interactions satisfying:

$V_{FF}/V_{BF} = V_{BF}/V_{BB} = 1.5, \quad V_{BB}/U = 1/10.$

- *Bose-Fermi Solid* phase with gapped pseudo-spin and pseudo-charge excitations
- *Bose-Fermi Mott* phase with gapped pseudo-charge excitation
- *Bose-Fermi Liquid* phase with gapless excitations in both sectors
- Intermediate phases near the boundaries
- *Bose-Fermi Solid* can melt through different processes, depending on whether fermion-fermion or boson-boson NN interaction is more dominant. It manifests the important role of quantum statistics in the melting process of *Bose-Fermi Solid.*

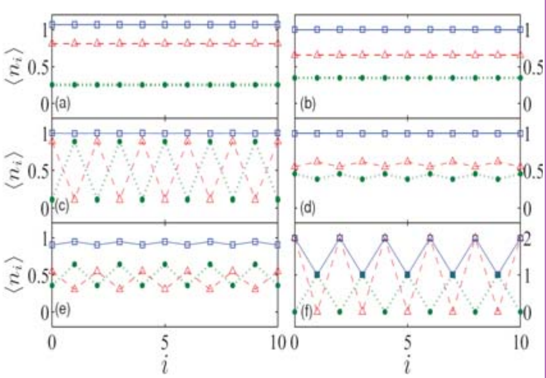

Fig. 2 Typical real-space density distributions of bosons (open triangles), fermions (solid dots), and bosons+fermions (open squares) for (a) Uniform BFL (b) UBFM (c) half-filled BFS (d) Density Wave-BFM (e) DW-BFL (f) BFS with higher filling

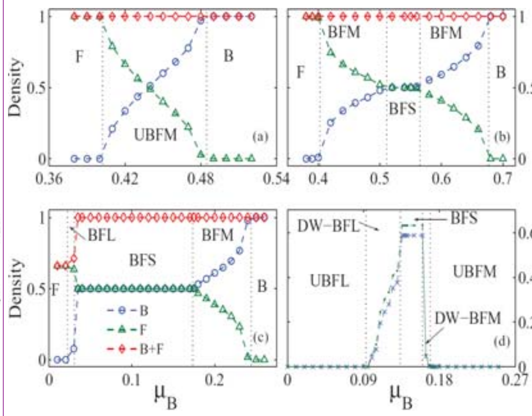

Fig.3 (a-c) Average boson, fermion, and boson+fermion density as functions of the boson chemical potential for the data points along the vertical dotted lines at J=0.1U in Fig. 1 (a-c));
(d) $|\langle n_i^B\rangle - \langle n_{i+1}^B\rangle|$ and $|\langle n_i^F\rangle - \langle n_{i+1}^F\rangle|$ for the data points along the vertical dotted line at J=0.17U in Fig. 1 (c), which characterize the charge density order.

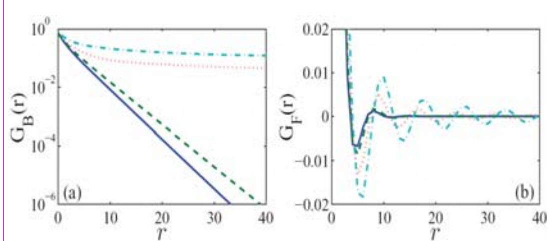

Fig. 4 Single particle Green's function. In the Bose-Fermi Mott phase (solid and dashed curves), the correlation functions decay exponentially, while they show a slower algebraic decay behavior due to the quasi-long-ranged order in the Bose-Fermi Liquid phase (dotted and dash-dotted curves).

Conclusion

In summary, we studied the ground-state phase diagram of the Bose-Fermi Hubbard model with arbitrary NN interactions. We discover the possibility and the condition to find a novel Bose-Fermi solid phase, which has a nontrivial quantum melting due to the mixture of quantum statistics even in 1D.

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