Phase Diagram of Boson-Fermion Mixtures in Optical Lattices

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Overview & Summary

- recent experiments on the Mott-insulator transition for bosonic atoms in optical lattices [1] reveal the huge potential of this new class of systems for the study of quantum phase transitions
- atomic boson-fermion mixtures in optical lattices [2] offer unique possibilities to investigate quantum phase transitions in mixed statistics systems, which are hard to access in the solid state context
- we utilise the Bose-Fermi-Hubbard model [3-6] to describe boson-fermion mixtures at zero temperature via an exact numerical solution of the eigenvalue problem
- the stiffness of the system under phase variations is used to obtain information on the superfluid density of the bosonic species and the conductivity of the fermionic component [6-8]
- two completely insulating phases are found (besides the bosonic Mott insulator) which exist for all filling factors: one exhibits diagonal long-range order through an alternating boson/fermion occupation, the other shows an intrinsic phase separation
- the pronounced correlations within these phases become manifest in the two-body density matrix as well as in the static structure factor

Bose-Fermi-Hubbard Model

- one-dimensional lattice with I sites, N_B bosons, and N_F fermions
- single-band **Bose-Fermi-Hubbard Hamiltonian** with nearest neighbour hopping and on-site boson-boson and boson-fermion interactions [3-6]:

$$\hat{\mathrm{H}} = -J_\mathrm{B}\sum_{i=1}^{I}(\hat{\mathrm{a}}_{i+1}^\dagger \hat{\mathrm{a}}_i + \mathrm{h.a.}) - J_\mathrm{F}\sum_{i=1}^{I}(\hat{\mathrm{c}}_{i+1}^\dagger \hat{\mathrm{c}}_i + \mathrm{h.a.}) \qquad \textbf{hopping terms}$$

$$+\frac{V_\mathrm{BB}}{2}\sum_{i=1}^{I}\hat{\mathrm{n}}_i^\mathrm{B}(\hat{\mathrm{n}}_i^\mathrm{B}-1) + V_\mathrm{BF}\sum_{i=1}^{I}\hat{\mathrm{n}}_i^\mathrm{B}\hat{\mathrm{n}}_i^\mathrm{F} \qquad \textbf{two-body interactions}$$

$\hat{\mathrm{a}}_i^\dagger$, $\hat{\mathrm{c}}_i^\dagger$	creation operators for boson/fermion at site i
$\hat{\mathrm{n}}_i^\mathrm{B}$, $\hat{\mathrm{n}}_i^\mathrm{F}$	boson/fermion occupation number operators for site i
J_B, J_F	tunnelling matrix element between adjacent sites
V_BB, V_BF	on-site boson-boson/boson-fermion interaction strength

- states represented in a **complete basis of Fock states** $|n_1^\mathrm{B},...,n_I^\mathrm{B}\rangle \otimes |n_1^\mathrm{F},...,n_I^\mathrm{F}\rangle$ with all allowed sets of occupation numbers with $\sum_i n_i^\mathrm{B} = N_\mathrm{B}$ and $\sum_i n_i^\mathrm{F} = N_\mathrm{F}$

$$|\Psi_0\rangle = \sum_{\alpha=1}^{D_\mathrm{B}}\sum_{\beta=1}^{D_\mathrm{F}} C_{\alpha\beta}\, |\{n_1^\mathrm{B},...,n_I^\mathrm{B}\}_\alpha\rangle \otimes |\{n_1^\mathrm{F},...,n_I^\mathrm{F}\}_\beta\rangle$$

- **exact solution** of large-scale eigenvalue problem for a few eigenstates with Lanczos-type algorithm; basis dimensions up to $D = D_\mathrm{B} D_\mathrm{F} \approx 10^6$ feasible [6]
- simple quantities—like mean occupation numbers, number fluctuations, energy gap E_gap, or one- and two-body density matrices—can be computed directly

Transport Properties

- the **stiffness under phase twists** is an important indicator for fundamental dynamical properties of the system [6-8]
- we impose a linear phase variation on either the bosonic or the fermionic component through Peierls phase factors in the respective hopping term

$$\hat{\mathrm{a}}_{i+1}^\dagger \hat{\mathrm{a}}_i \to \mathrm{e}^{-\mathrm{i}\Theta_\mathrm{B}/I}\,\hat{\mathrm{a}}_{i+1}^\dagger \hat{\mathrm{a}}_i \qquad \hat{\mathrm{c}}_{i+1}^\dagger \hat{\mathrm{c}}_i \to \mathrm{e}^{-\mathrm{i}\Theta_\mathrm{F}/I}\,\hat{\mathrm{c}}_{i+1}^\dagger \hat{\mathrm{c}}_i$$

- the phase twist causes an increase of the ground state energy; the energy change is connected to the kinetic energy of the flow generated by the phase gradient
- **boson twist**: the energy change resulting from a phase twist for the bosons is a measure for the superfluid density of the bosonic component; the stiffness can be identified with the **superfluid fraction** f_s^B (neglecting the suppression of the superfluid flow by the lattice itself) [6-8]

$$f_\mathrm{s}^\mathrm{B} = \frac{I^2}{N_\mathrm{B}}\,\frac{E_{\Theta_\mathrm{B}} - E_0}{J_\mathrm{B}\,\Theta_\mathrm{B}^2} \qquad \Theta_\mathrm{B} \ll \pi$$

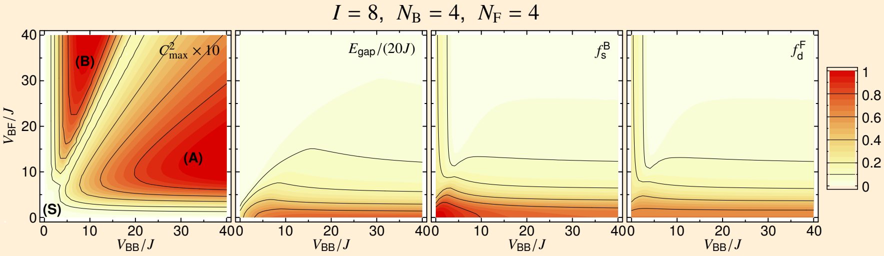
- **fermion twist**: the energy change resulting from fermionic phase twist is related to the conductivity of the fermionic component; the corresponding stiffness defines the **Drude weight** f_d^F which is related to the conductivity [6]

$$f_\mathrm{d}^\mathrm{F} = \frac{I^2}{N_\mathrm{F}}\,\frac{E_{\Theta_\mathrm{F}} - E_0}{J_\mathrm{F}\,\Theta_\mathrm{F}^2} \qquad \Theta_\mathrm{F} \ll \pi$$

- an important further step is the distinction between normal- and superconductivity for the fermionic component (work in progress)

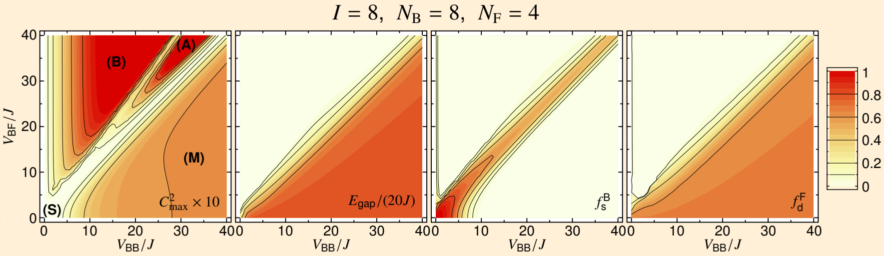
Phase Diagrams

$I = 8,\ N_\mathrm{B} = 4,\ N_\mathrm{F} = 4$



- subtle interplay between repulsive boson-boson and boson-fermion interactions and kinetic energy generates rich phase diagram [3-6]
- **(S) superfluid/conducting**: non-vanishing bosonic superfluidity and fermionic conductivity
- **(M) bosonic Mott-insulator**: vanishing boson superfluid fraction; fermionic component not affected and still conducting
- **(A) alternating occupation**: dominant basis states exhibit alternating boson-fermion occupation; diagonal long-range order; vanishing stiffness for both species
- **(B) block separation**: dominant basis states show separated blocks of bosons and fermions; vanishing stiffness for both species; kinetic energy governs the crossover (A) ↔ (B)

$I = 8,\ N_\mathrm{B} = 8,\ N_\mathrm{F} = 4$



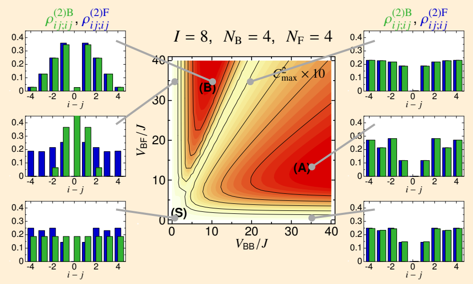
Two-Body Correlations

- important information on the intrinsic structure and correlations within the ground state is provided by the diagonal elements of the **two-body density matrix**

bosons $\quad \rho_{ij;ij}^{(2)\mathrm{B}} = \langle\Psi_0|\,\hat{\mathrm{a}}_i^\dagger \hat{\mathrm{a}}_j^\dagger \hat{\mathrm{a}}_j \hat{\mathrm{a}}_i\,|\Psi_0\rangle$

fermions $\quad \rho_{ij;ij}^{(2)\mathrm{F}} = \langle\Psi_0|\,\hat{\mathrm{c}}_i^\dagger \hat{\mathrm{c}}_j^\dagger \hat{\mathrm{c}}_j \hat{\mathrm{c}}_i\,|\Psi_0\rangle$

- $\rho_{ij;ij}^{(2)}$ describes the probability of finding two atoms at a distance $i-j$ (cyclic boundary conditions).
- **(A) alternating occupation**: probability of finding a pair of bosons/fermions at even $i-j$ is enhanced compared to odd $i-j$ ➔ **diagonal long-range order**
- **(B) block separation**: large probability for pairs at neighbouring sites (small $i-j$); probability decreases monotonically with increasing $i-j$
- these correlations can be detected experimentally through the static structure factor $S(q)$



contributed by *M. Hild & F. Schmitt*

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