Quantum phases of 1D Hubbard models with three- and four-body couplings

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The experimental advances in cold atomic and molecular gases stimulate the investigation of lattice correlated systems beyond the conventional on-site Hubbard approximation, by possibly including multi-particle processes. We study fermionic extended Hubbard models in a one dimensional lattice with different types of particle couplings, including also three- and four-body interaction up to nearest neighboring sites. By using the Bosonization technique, we investigate the low-energy regime and determine the conditions for the appearance of ordered phases, for arbitrary particle filling. We find that three- and four-body couplings may significantly modify the phase diagram. In particular, diagonal three-body terms that directly couple the local particle densities have qualitatively different effects from off-diagonal three-body couplings originating from correlated hopping, and favor the appearance of a Luther-Emery phase even when two-body terms are repulsive. Furthermore, the four-body coupling gives rise to a rich phase diagram and may lead to the realization of the Haldane insulator phase at half-filling.

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The Hubbard model at 50

editorial

The Hubbard model at half a century

Models are abundant in virtually all branches of physics, with some achieving iconic status. The Hubbard model, celebrating its golden jubilee this year, continues to be one of the most popular contrivances of theoretical condensed-matter physics.

$$H = -t \sum_{j=1}^{N_s} \sum_{\sigma} \left(c^{\dagger}_{j,\sigma} c_{j+1,\sigma} + \mathrm{h.c.} \right) + U \sum_{j=1}^{N_s} \hat{n}_{j\uparrow} \hat{n}_{j\downarrow}$$

Hubbard’s original motivation: Ferromagnetism in transition metals

Theoretical solution:
- Exactly solvable in 1D
- Numerical approximations in 2D, 3D using DMFT and DMRG

Today’s main uses:
- High-T_c superconductivity
- Atoms in optical lattices

[1] Nat. Phys. **9**, 523 (2013)
[2] Gutzwiller, M. C. Phys. Rev. Lett. **10**, 159 (1963).
[3] Kanamori, J. Prog. Theor. Phys. **30**, 275 (1963).
[4] Hubbard, J. Proc. R. Soc. A **276**, 237 (1963)

Hamiltonian

The extended (``all you can eat'') Hubbard model:

3-particle interaction (off-diagonal)

NN hopping

Correlated hopping

$$H = \sum_{j=1}^{N_s} \Big[-\sum_{\sigma} (c^\dagger_{j,\sigma} c_{j+1,\sigma} + \text{h.c.})[t - X(\hat{n}_{j\bar{\sigma}} + \hat{n}_{j+1\bar{\sigma}}) + \tilde{X} \hat{n}_{j\bar{\sigma}} \hat{n}_{j+1\bar{\sigma}}]$$

$$+ U \hat{n}_{j\uparrow} \hat{n}_{j\downarrow}$$ onsite interaction

$$+ V \hat{n}_j \hat{n}_{j+1}$$ NN interaction

$$+ J \mathbf{S}_j \cdot \mathbf{S}_{j+1}$$ Spin exchange

$$+ Y (c^\dagger_{j\uparrow} c^\dagger_{j\downarrow} c_{j+1\downarrow} c_{j+1\uparrow} + \text{h.c.})$$ Pair hopping

$$+ P (\hat{n}_{j\uparrow} \hat{n}_{j\downarrow} \hat{n}_{j+1} + \hat{n}_{j+1\uparrow} \hat{n}_{j+1\downarrow} \hat{n}_j)$$ 3-particle interaction (diagonal)

$$+ Q\, \hat{n}_{j\uparrow} \hat{n}_{j\downarrow} \hat{n}_{j+1\uparrow} \hat{n}_{j+1\downarrow} \Big]$$ 4-particle interaction

8 Parameters: $X, \tilde{X}, U, V, J, Y, P, Q$

Symmetries:
- Charge $U(1)$
- Spin $SU(2)$
- Discrete lattice translation

$$\hat{n}_{j\sigma} = c^\dagger_{j\sigma} c_{j\sigma}$$

$$\hat{n}_j = \hat{n}_{j\uparrow} + \hat{n}_{j\downarrow}$$

$$\mathbf{S}_j = \sum_{\sigma\sigma'} (c^\dagger_{j\sigma} \vec{\sigma}_{\sigma\sigma'} c_{j\sigma'})/2$$

Bosonization

Assumptions:

- Weak coupling regime (all constants $\ll t$)
- Linearization of the spectrum around $\pm k_F(\rho)$
- Continuum limit

$$c_{j\sigma}^\dagger \to \sqrt{a}\left(e^{-ik_F x} R_\sigma^\dagger(x) + e^{+ik_F x} L_\sigma^\dagger(x)\right)$$

6 Parameters:
K_ν, v_ν, m_ν
depend on all couplings and filling factor ρ

Bosonization:

$$R_\sigma^\dagger(x) = \frac{\kappa_{R\sigma}}{\sqrt{2\pi\alpha}} \exp\left[-i\sqrt{4\pi}\,\frac{\Phi_\sigma(x) + \Theta_\sigma(x)}{2}\right]$$

$$L_\sigma^\dagger(x) = \frac{\kappa_{L\sigma}}{\sqrt{2\pi\alpha}} \exp\left[+i\sqrt{4\pi}\,\frac{\Phi_\sigma(x) - \Theta_\sigma(x)}{2}\right]$$

Result:

- Spin and charge modes: $\Phi_{\uparrow,\downarrow}(x) \to \Phi_{c/s}(x) = (\Phi_\uparrow \pm \Phi_\downarrow)/\sqrt{2}$
- Spin-charge separation $H = H_c + H_s$
- Decoupled sine-Gordon Hamiltonians:

$$H_\nu = \frac{\hbar v_\nu}{2} \int dx \left[\sqrt{K_\nu} : (\partial_x \Theta_\nu)^2 : + : (\partial_x \Phi_\nu)^2 : / \sqrt{K_\nu} + \frac{m_\nu}{2\pi\alpha^2} \cos\left(\sqrt{8\pi}\Phi_\nu(x)\right)\right]$$

Wait a second…

Operator product expansion

Operator product expansion (OPE):

$$\langle \phi_i(r_1)\phi_j(r_2)\Phi\rangle \approx \sum_j C_{ijk}(r_1 - r_2)\,\langle \phi_k(r_1)\Phi\rangle$$

- $C_{ijk}(r)$ depends only on scaling dimensions, not on Φ

$$C_{ijk}(r) = \frac{c_{ijk}}{|r|^{x_i + x_j - x_k}}$$

- Useful for RG in conformal invariant systems

Here, OPEs are used directly on the Hamiltonian (small lattice spacing):

$$\frac{e^{\pm i\sqrt{4\pi}\Phi_\sigma(x)}e^{\mp i\sqrt{4\pi}\Phi_\sigma(x+a)}}{(2\pi\alpha)^2} \simeq \frac{1}{(2\pi a)^2} \mp i\frac{\partial_x\Phi_\sigma}{2\pi^{3/2}a} - \frac{:(\partial_x\Phi_\sigma)^2:}{2\pi} \mp \frac{i\partial_x^2\Phi_\sigma}{4\pi^{3/2}}$$

$$\frac{\partial_x\Phi_\sigma(x)}{\sqrt{\pi}}\,\frac{e^{\pm i\sqrt{4\pi}\Phi_\sigma(x+a)}}{2\pi\alpha} \simeq \pm\frac{i\,e^{\pm i\sqrt{4\pi}\Phi_\sigma(x)}}{2\pi^2 a\,\alpha} - \frac{:e^{\pm i\sqrt{4\pi}\Phi_\sigma(x)}\partial_x\Phi_\sigma(x):}{L\sqrt{\pi}}$$

$$\frac{e^{\pm i\sqrt{4\pi}\Phi_\sigma(x)}}{2\pi\alpha}\,\frac{\partial_x\Phi_\sigma(x+a)}{\sqrt{\pi}} \simeq \mp\frac{i\,e^{\pm i\sqrt{4\pi}\Phi_\sigma(x)}}{2\pi^2 a\,\alpha} + \frac{:e^{\pm i\sqrt{4\pi}\Phi_\sigma(x)}\partial_x\Phi_\sigma(x):}{L\sqrt{\pi}}$$

Only derivatives and cosine terms remain
→ Sine-Gordon Hamiltonian

Renormalization group

$$H_\nu = \frac{\hbar v_\nu}{2}\int dx[\sqrt{K_\nu} :(\partial_x\Theta_\nu)^2: + :(\partial_x\Phi_\nu)^2: /\sqrt{K_\nu} + \frac{m_\nu}{2\pi\alpha^2}\cos(\sqrt{8\pi}\Phi_\nu(x))] \qquad (\nu = c, s)$$

Weak coupling analysis:

$$K_\nu \approx 1$$
$$m_\nu \ll 1$$

Perturbative RG equations:

$$\frac{d\xi_\nu}{dl} = -m_\nu^2, \qquad \frac{dm_\nu}{dl} = -\xi_\nu m_\nu, \qquad \xi_\nu = 4\left(\sqrt{K_\nu} - 1\right)$$

Gap opens if m_ν flows to strong coupling

Charge sector:

- K_c and m_c are independent
- Charge gap can occur both for $m_c > 0$ and $m_c < 0$
- Only at half filling

Spin sector:

- K_s and m_s are connected by $SU(2)$ symmetry:

$$K_s \approx 1 + m_s/2$$

- Spin gap only for $m_s < 0$

Δ_c	Δ_s	$\sqrt{2\pi}\Phi_c$	$\sqrt{2\pi}\Phi_s$	Type of Phase
$=0$	$=0$	fluctuating	fluctuating	LL
$=0$	$\neq 0$	fluctuating	πp_s	LE
$\neq 0$	$=0$	πp_c	fluctuating	MI
$\neq 0$	$=0$	$\pi(p_c + 1/2)$	fluctuating	HI
$\neq 0$	$\neq 0$	πp_c	πp_s	BOW
$\neq 0$	$\neq 0$	$\pi(p_c + 1/2)$	πp_s	CDW

$p_\nu \in \mathbb{Z}$

Long-range order

Parity and string operators: (Non-local)

$$O_P^{(\nu)}(j) = \prod_{l=1}^{j} e^{i\pi J_l^{(\nu)}}$$

$$O_S^{(\nu)}(j) = J_j^{(\nu)} \prod_{l=1}^{j} e^{i\pi J_l^{(\nu)}}$$

$$J_l^{(c)} = \hat{n}_l - 1$$

$$J_l^{(s)} = (\hat{n}_{l,\uparrow} - \hat{n}_{l,\downarrow})$$

$$J_l^{\nu} \in \{-1, 0, 1\}$$

Correlation functions:

$$C_P^{(\nu)}(r) = \langle O_P^{(\nu)}(j) O_P^{(\nu)\dagger}(j+r)\rangle$$
$$\sim \langle \cos[\sqrt{2\pi}\Phi_\nu(0)]\cos[\sqrt{2\pi}\Phi_\nu(x)]\rangle$$

$$C_S^{(\nu)}(r) \sim \langle \sin[\sqrt{2\pi}\Phi_\nu(0)]\sin[\sqrt{2\pi}\Phi_\nu(x)]\rangle$$

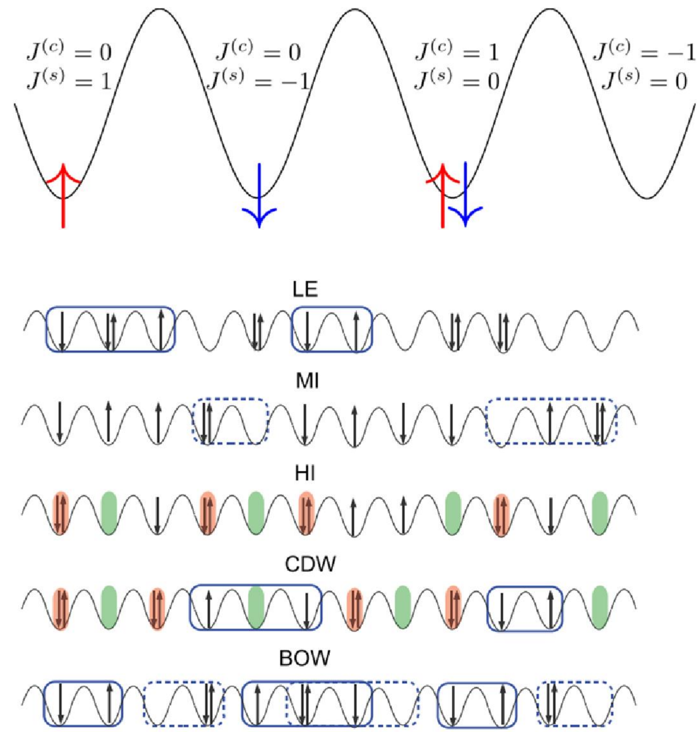


FIG. 1. (Color online) Cartoon illustrating the possible orders in presence of fluctuations. The blue continuous (dashed) lines show the correlated pairs of up-down spin (holon-doublon) allowing $\langle O_P^{(s)}\rangle$ ($\langle O_P^{(c)}\rangle$) to remain nonvanishing. The green and red circles show the alternation of sites occupied by doublons and holons in the chain of single fermions preserving $\langle O_S^{(c)}\rangle \neq 0$.

	Δ_c	Δ_s	LRO
LL	0	0	none
LE	0	open	$O_P^{(s)}$
MI	open	0	$O_P^{(c)}$
HI	open	0	$O_S^{(c)}$
BOW	open	open	$O_P^{(c)}$, $O_P^{(s)}$
CDW	open	open	$O_S^{(c)}$, $O_P^{(s)}$

Long-range order (LRO):

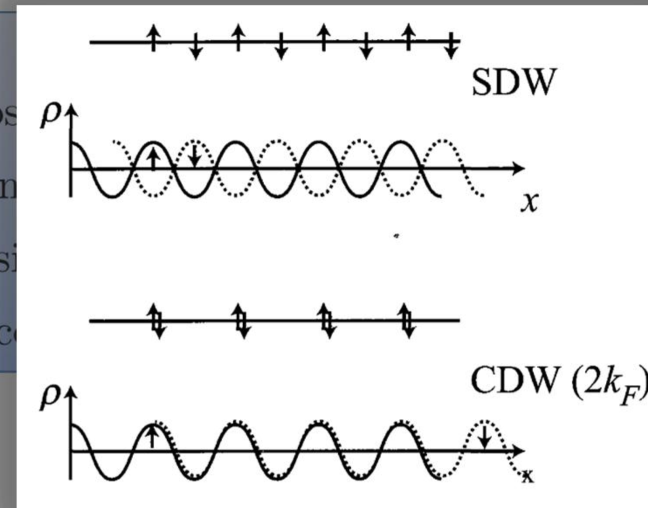
$$\left\langle C_P^{(\nu)}(r) C_P^{(\nu)}(0) \right\rangle \to \text{const. for } r \to \infty$$

from: Barbiero *et al.*, PRB **88**, 035109 (2013)

Possible phases

Local order parameters:

- Charge density wave: $O_{CDW}(x) = \sin[\sqrt{2\pi}\Phi_c(x)]$ cos
- Spin density wave: $O_{SDW}(x) = \cos[\sqrt{2\pi}\Phi_c(x)]$ sin
- Singlet superconductivity: $O_{TS}(x) = \exp[i\sqrt{2\pi}\Theta_c(x)]$ si
- Triplet superconductivity: $O_{SS}(x) = \exp[i\sqrt{2\pi}\Theta_c(x)]$ c



Phases at half filling:

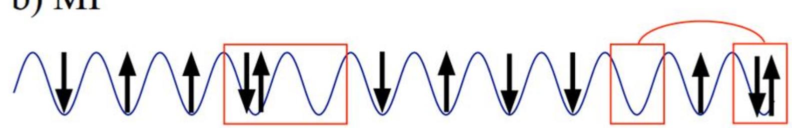
Luttinger liquid (LL):
- Gapless in charge and spin sector
- Attractive interactions: $K_c^* > 1$
- Dominant correlation function:
  $\langle O_{TS}(x) O^\dagger_{TS}(y)\rangle \sim |x-y|^{-(1+K_c^*)}$

Luther-Emery liquid (LE):
- Gapless charge sector
- Gapped spin sector
- CDW and SS order:
  $\langle O_{CDW,SS}(x) O^\dagger_{CDW,SS}(y)\rangle \sim |x-y|^{-1/K_c^*}$

Charge insulator:
- Mott insulator (MI):
  $\langle O_{SDW}(x) O^\dagger_{SDW}(y)\rangle \sim |x-y|^{-1}$
- Haldane insulator (HI):
  $\langle O_{CDW}(x) O^\dagger_{CDW}(y)\rangle \sim |x-y|^{-1}$

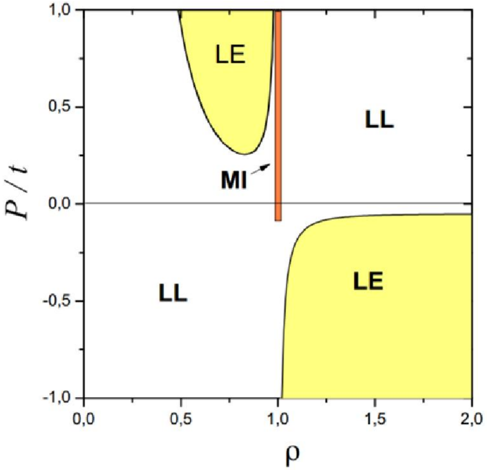
Fully gapped phases:
- CDW and BOW (bond ordered wave) phases

b) MI

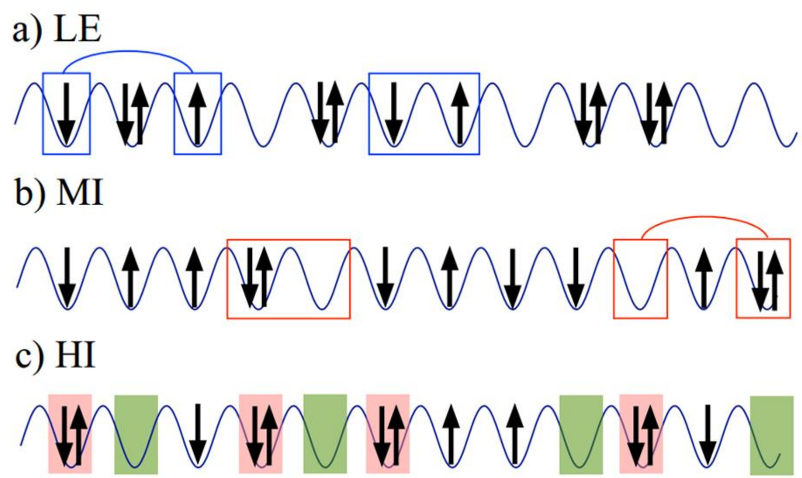


Three-particle interaction

$U = 3V = t/4$

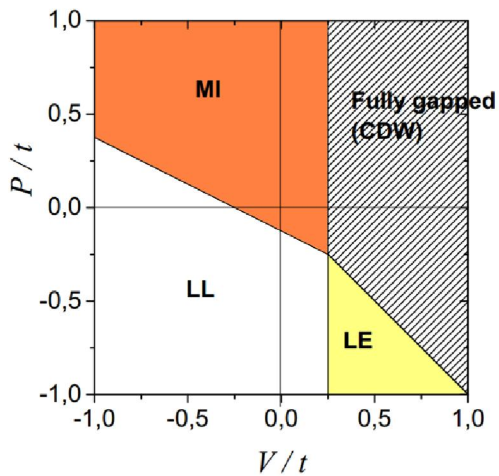


$P\hat{n}_{j\uparrow}\hat{n}_{j\downarrow}\hat{n}_{j+1}$



Half filling ($\rho = 1$)

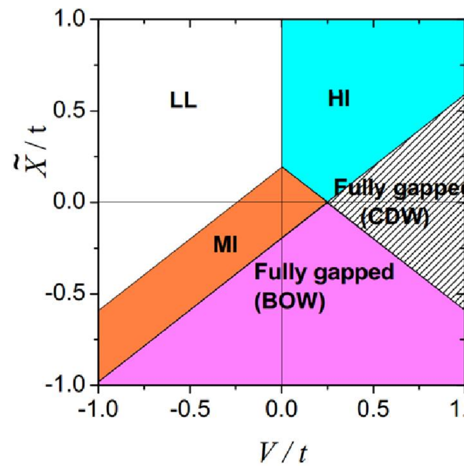
$U = t/2$



$P\hat{n}_{j\uparrow}\hat{n}_{j\downarrow}\hat{n}_{j+1}$

Three-body terms:

- Off-diagonal: HI phase
- Diagonal: LE phase

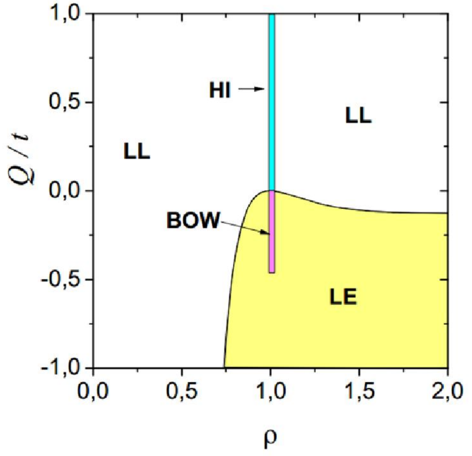


$\tilde{X}c^{\dagger}_{j,\sigma}c_{j+1,\sigma}\hat{n}_{j\bar{\sigma}}\hat{n}_{j+1\bar{\sigma}}$

Four-particle interaction

For general filling:
Transition between LE and LL for $Q < 0$

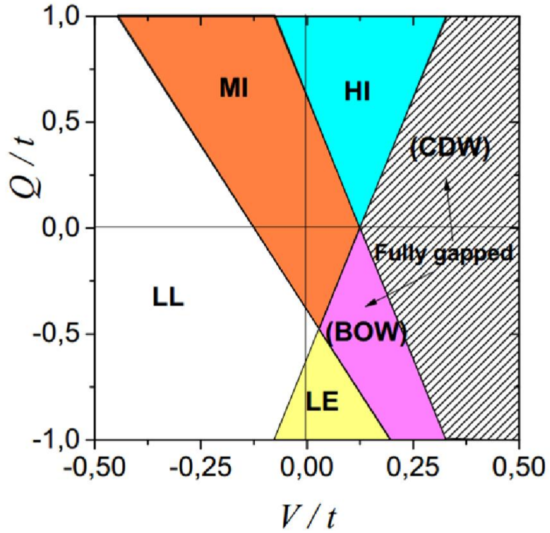
$U = 2V = t$



At half filling ($\rho = 1$):

- All phases can be realized as function of V and Q
- Repulsive $Q > 0$ favors HI, whereas repulsive $U > 0$ favors MI
- No off-diagonal terms necessary for HI

$U = t/4$



Conclusions

- The phases of the extended Hubbard model can be classified with nonlocal spin and charge order parameters.

- Depending on gaps opening in spin and charge sectors, various phases may emerge:
  - Luther-Emery,
  - Mott insulator, Haldane insulator,
  - Charge density wave, Bond ordered wave

- Three- and four-particle interaction terms may be convenient to explore these phases in cold atom systems

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