Phase Diagrams in one-dimensional fermion system

Hamid Mosadeq
SKU & IPM

Experimental realization of 1D system

- Polymers
- Organic compounds
- Bulk materials with one-dimensional structure inside
  - Ladder compounds
  - spin compounds
- Nano-materials
  - quantum wire
  - Josephson junction array
  - edge state in quantum Hall systems
  - nanotubes
- Ultracold atoms in optical lattices

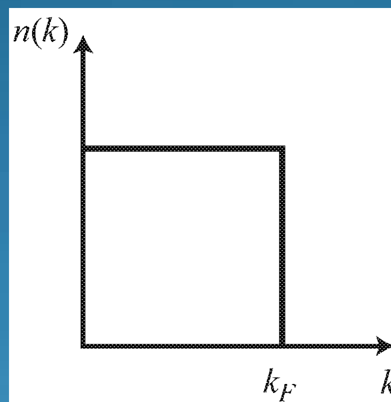
S. Roth, D. Caroll, "One-Dimensional Metals", WILEY (2004)
R.T. Piil. "Cold atoms in one-dimensional periodic potentials", Phd Thesis (2008)

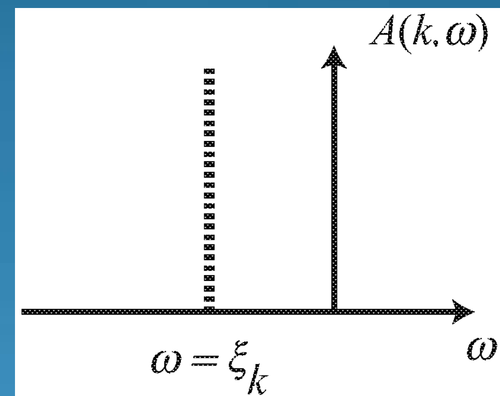
Peculiarities of 1D

The effect of interaction in high-dimension: Fermi liquid theory

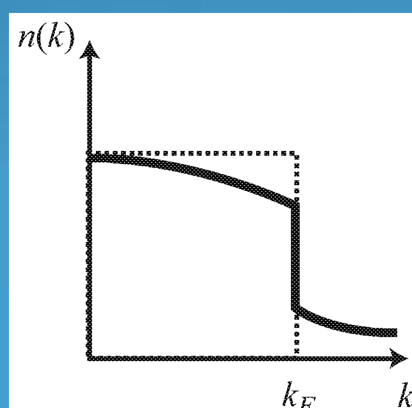
A caricature of theory

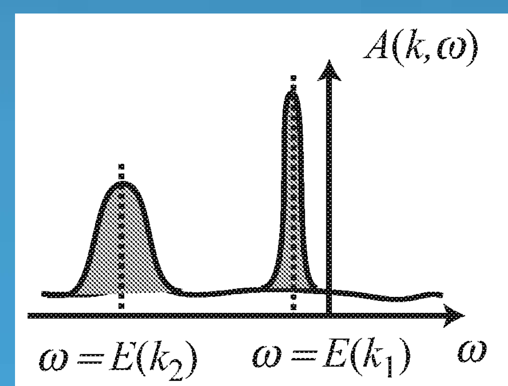
Free electrons





When interactions are switched on



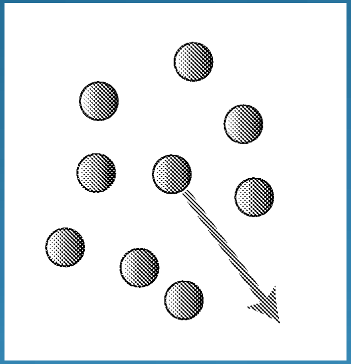


T. Giamarchi, “Quantum Physics in One Dimension”, Oxford(2003)

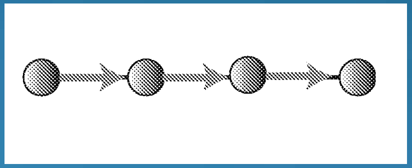
Peculiarities of 1D

Crash course on Fermi liquids

A major different: Collectivization of excitations



nearly free quasi-particle excitations



Collective excitation

Failure perturbation theory

How to solve

Bosonization method

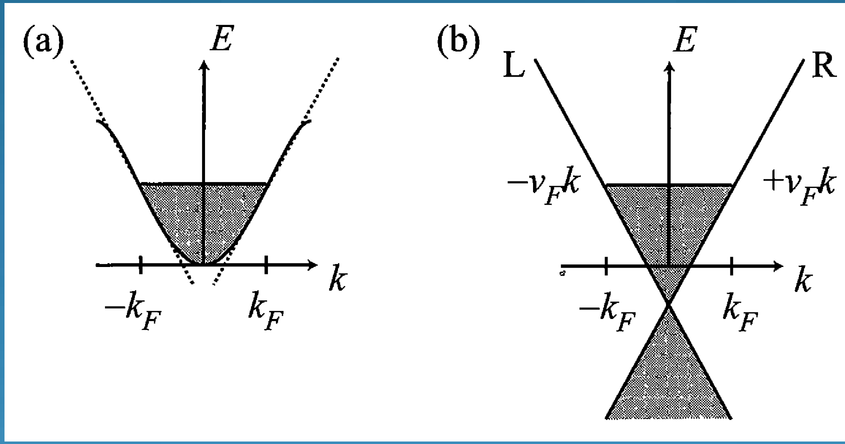
Fermionic method

T. Giamarchi, “Quantum Physics in One Dimension”, Oxford(2003)

Bosonization

Low energy properties of 1D systems

Spinless model: representation of excitations



The Hamiltonian of system $H = \sum_{k;r=R,L} v_F(\epsilon_r k - k_F) c^\dagger_{r,k} c_{r,k}$

The particle-hole excitations $E_{R,k}(q) = v_F(k+q) - v_F k = v_F q$

The density fluctuations $\rho^\dagger(q) = \sum_k c^\dagger_{k+q} c_k$

T. Giamarchi, "Quantum Physics in One Dimension", Oxford(2003)

Bosonization

Low energy properties of 1D systems

Spinless model: representation of excitations

The boson creation and destruction operator

$$b_p^\dagger = \left(\frac{2\pi}{L|p|}\right)^{1/2} \sum_r Y(rp)\rho_r^\dagger(p)$$

$$b_p = \left(\frac{2\pi}{L|p|}\right)^{1/2} \sum_r Y(rp)\rho_r^\dagger(-p)$$

$$\phi(x), \theta(x) = \mp(N_R \pm N_L)\frac{\pi x}{L} \mp \frac{i\pi}{L} \sum_{p\neq 0} \frac{1}{p} e^{-\alpha|p|/2 - ipx}(\rho_R^\dagger(p) \pm \rho_L^\dagger(p))$$

$$\Pi(x) = \frac{1}{\pi}\nabla\theta(x)$$

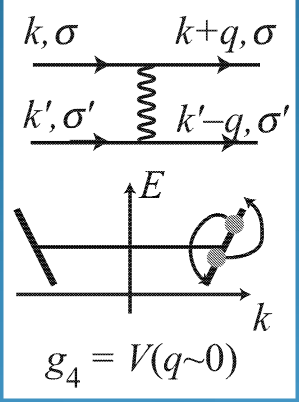
T. Giamarchi, "Quantum Physics in One Dimension", Oxford(2003)

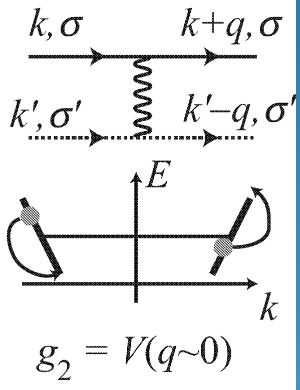
Bosonization

Low energy properties of 1D systems

Spinless model: representation of excitations

$$\psi(x) \simeq \frac{1}{\sqrt{\Omega}} \left[\sum_{-\Lambda<k-k_F<\Lambda} e^{ikx} c_k + \sum_{-\Lambda<k+k_F<\Lambda} e^{ikx} c_k \right]$$





$$\frac{g_4}{2}\psi_R^\dagger(x)\psi_R(x)\psi_R^\dagger(x)\psi_R(x) = \frac{g_4}{2}\rho_R(x)\rho_R(x) = \frac{g_4}{2}\frac{1}{(2\pi)^2}(\nabla\phi - \nabla\theta)^2$$

$$\begin{aligned} g_2\psi_R^\dagger(x)\psi_R(x)\psi_L^\dagger(x)\psi_L(x) &= g_2\rho_R(x)\rho_L(x) \\ &= \frac{g_2}{(2\pi)^2}(\nabla\phi - \nabla\theta)(\nabla\phi + \nabla\theta) \\ &= \frac{g_2}{(2\pi)^2}[(\nabla\phi)^2 - (\nabla\theta)^2] \end{aligned}$$

T. Giamarchi, "Quantum Physics in One Dimension", Oxford(2003)

Bosonization

Low energy properties of 1D systems

Spinless model: representation of excitations

The effective Hamiltonian of interacting fermions in one-dimension and near the Fermi surface

$$H = \frac{1}{2\pi} \int dx [uK(\pi\Pi(x))^2 + \frac{u}{K}(\nabla\phi(x))^2]$$

$$uK = v_F \left(1 + \frac{g_4}{2\pi v_F} - \frac{g_2}{2\pi v_F}\right)$$

$$\frac{u}{K} = \left(1 + \frac{g_4}{2\pi v_F} + \frac{g_2}{2\pi v_F}\right) v_F$$

The Physics of an interacting one-dimensional fermions is described by free bosonic excitations.

T. Giamarchi, "Quantum Physics in One Dimension", Oxford(2003)

Bosonization

Low energy properties of 1D systems

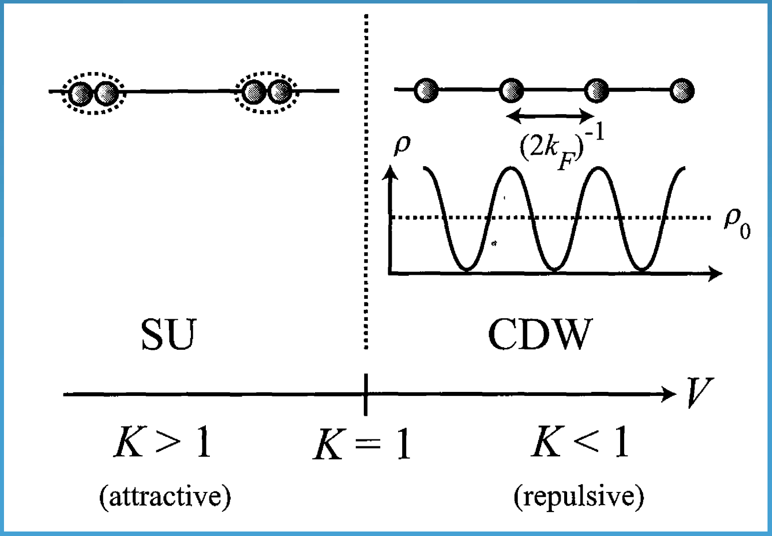
Spinless model: representation of excitations

The densiy-density correlation function

$$R_0(r) = \langle \rho(r)\rho(0)\rangle = \frac{K}{2\pi^2}\frac{y_\alpha^2 - x^2}{(x^2+y_\alpha^2)^2} + \frac{2}{(2\pi\alpha)^2}\cos(2k_F x)\left(\frac{\alpha}{r}\right)^{2K}$$

The superconducting correlation function

$$R_{\mathrm{SU}}(r) = \langle O_{\mathrm{SU}}(r) O_{\mathrm{SU}}^\dagger(0)\rangle = \frac{1}{(\pi\alpha)^2}\left(\frac{\alpha}{r}\right)^{1/(2K)}$$



Bosonization

Low energy properties of 1D systems

Model with spin; charge and spin excitations

The total charge and spin degree of freedom

$$\rho(x) = \frac{1}{\sqrt{2}}[\rho_\uparrow(x) + \rho_\downarrow(x)]$$

$$\sigma(x) = \frac{1}{\sqrt{2}}[\rho_\uparrow(x) - \rho_\downarrow(x)]$$

The new boson fields

$$\phi_\rho(x) = \frac{1}{\sqrt{2}}[\phi_\uparrow(x) + \phi_\downarrow(x)]$$

$$\phi_\sigma(x) = \frac{1}{\sqrt{2}}[\phi_\uparrow(x) - \phi_\downarrow(x)]$$

Using the spin-charge separation

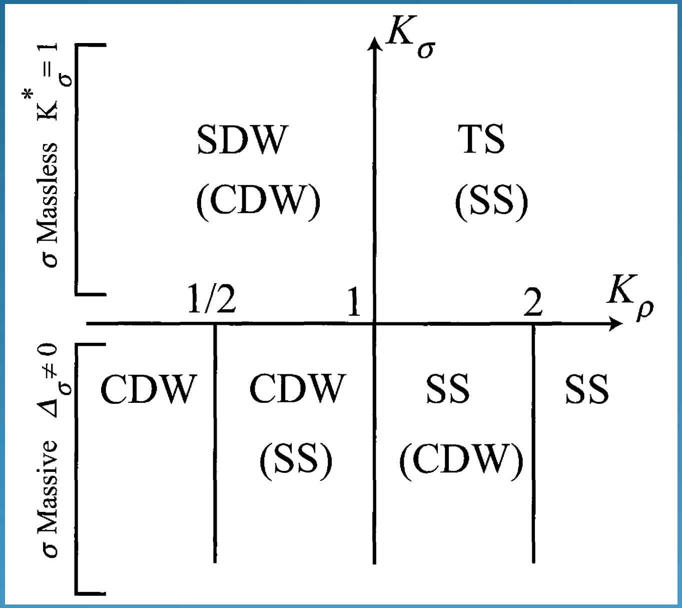
$$H = H_\rho + H_\sigma$$

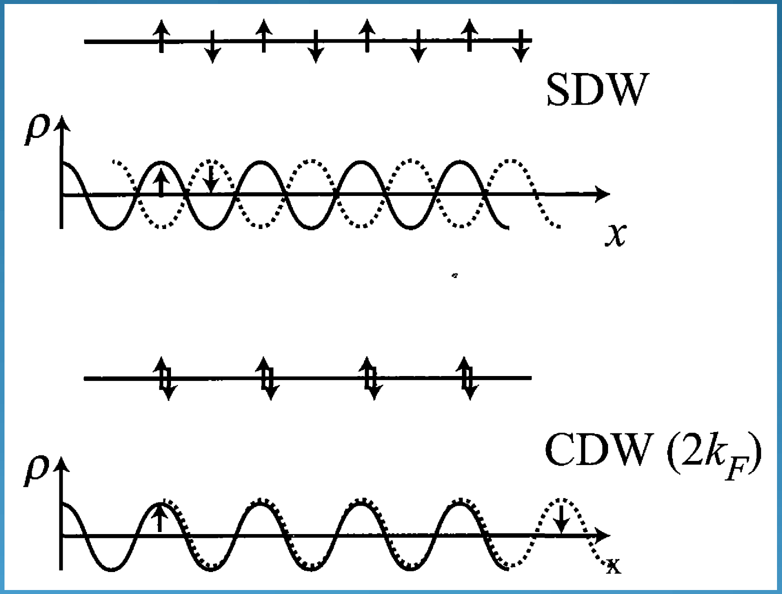
T. Giamarchi, “Quantum Physics in One Dimension”, Oxford(2003)

Bosonization

Low energy properties of 1D systems

Model with spin; charge and spin excitations





T. Giamarchi, "Quantum Physics in One Dimension", Oxford(2003)

Exact Diagonalization (ED)

The advantage

The simplest numerical method
Diagonalizes the full interacting Hamiltonian
Determines the eigenvalues and the eigenvectors

The drawback

The size limitation

Example

Spin-1/2 Heisenberg Model

Spin-1/2 Hubbard Model

Lanczoc (1950)

Density Matrix Renormalization Group (DMRG)

Real-space renormalization of Hamiltonians

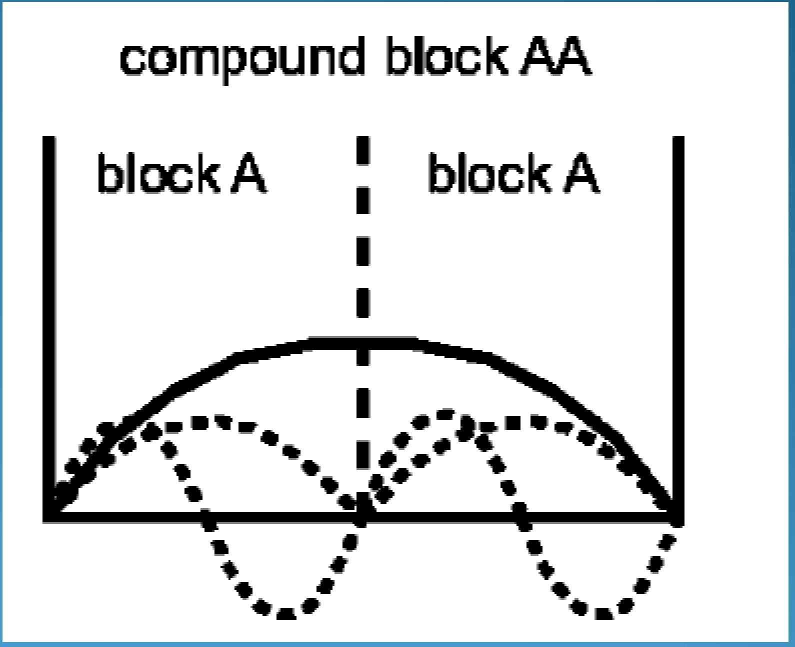
(1) Describe interactions on an initial sublattice ("block") A of length ℓ by a block Hamiltonian $\hat{H}_{\mathrm{A}}$ acting on an M-dimensional Hilbert space.

(2) Form a compound block AA of length 2ℓ and the Hamiltonian $\hat{H}_{\mathrm{AA}}$, consisting of two block Hamiltonians and interblock interactions. $\hat{H}_{\mathrm{AA}}$ has dimension M^2.

(3) Diagonalize $\hat{H}_{\mathrm{AA}}$ to find the M lowest-lying eigenstates.

(4) Project $\hat{H}_{\mathrm{AA}}$ onto the truncated space spanned by the M lowest-lying eigenstates, $\hat{H}_{\mathrm{AA}} \rightarrow \hat{H}^{\mathrm{tr}}_{\mathrm{AA}}$.

(5) Restart from step (2), with doubled block size: $2\ell \rightarrow \ell$, AA$\rightarrow$A, and $\hat{H}^{\mathrm{tr}}_{\mathrm{AA}} \rightarrow \hat{H}_{\mathrm{A}}$, until the box size is reached.

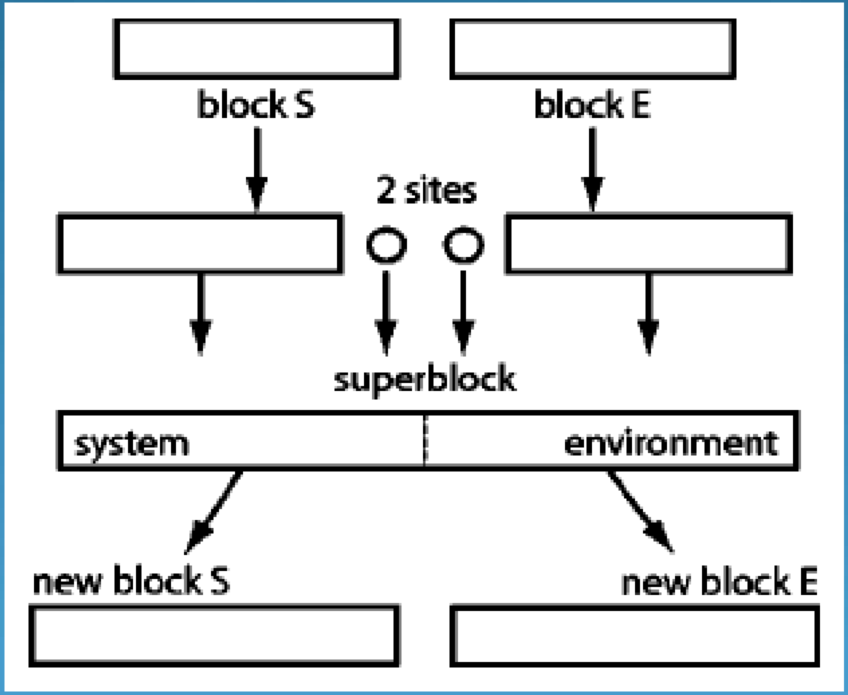


U. Scholwock, Rev. Mod. Phys(2005)

Density Matrix Renormalization Group (DMRG)

Density matrices and DMRG truncation

Infinite system DMRG



U. Scholwock, Rev. Mod. Phys(2005)

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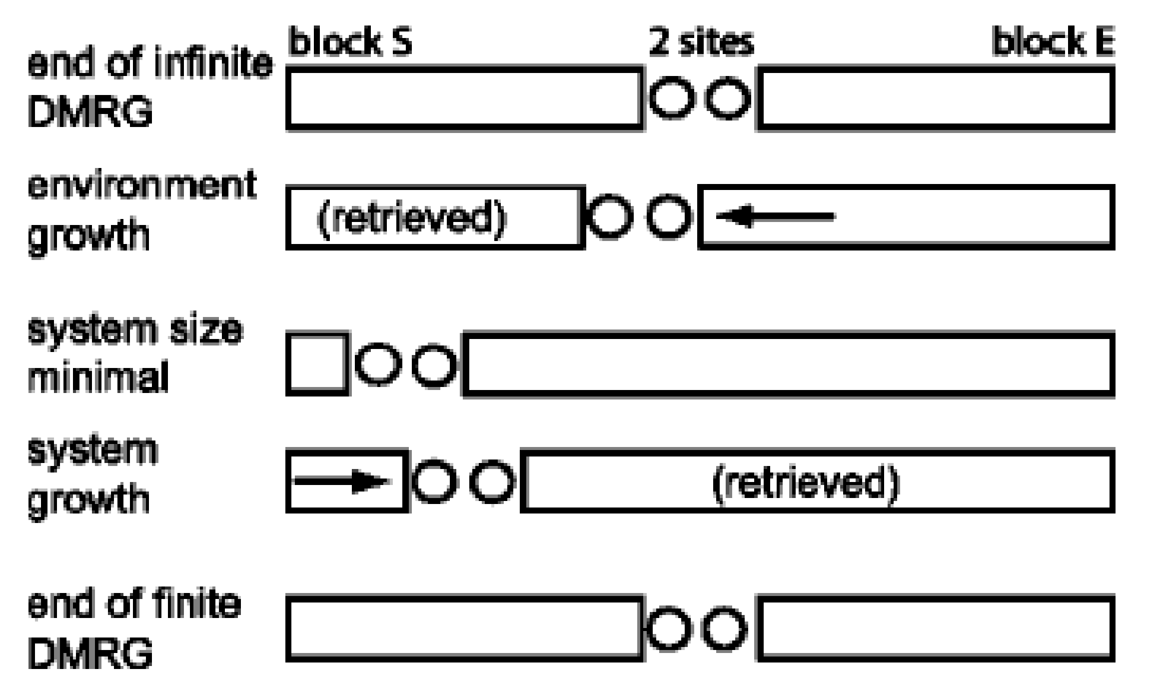


U. Scholwock, Rev. Mod. Phys(2005)

The **ALPS project** (**A**lgorithms and **L**ibraries for **P**hysics **S**imulations)

http://alps.com-phys.org/mediawiki/index.php/Main_Page

Monte Carlo

- Classical Monte Carlo
- Directed loop QMC
- worm QMC
- Directed worm

Exact Diagonalization

- Sparse Diagonalization(Lancsoz)
- Full Diagonalization

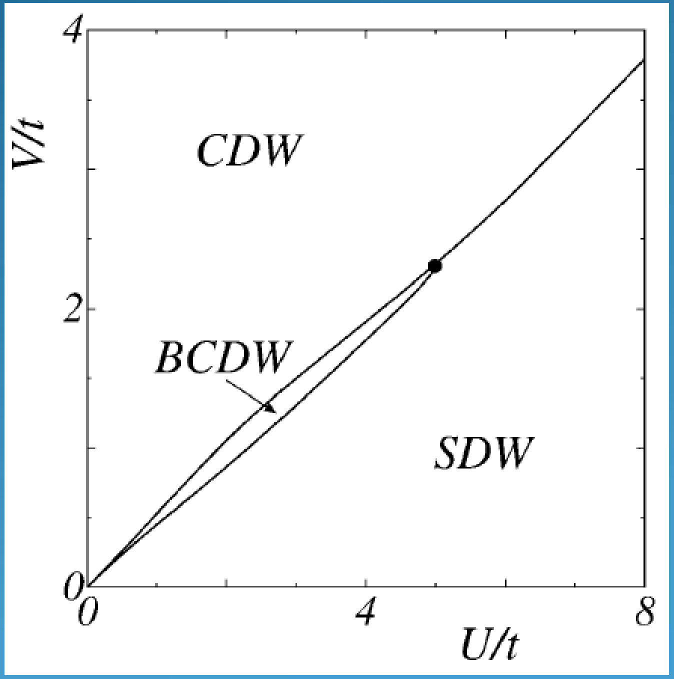
DMRG

DMFT

Extended Hubbard Model

At Half-filling

$$H = -t \sum_{\sigma=\uparrow,\downarrow} \sum_i (c^\dagger_{\sigma,i+1} c_{\sigma,i} + c^\dagger_{\sigma,i} c_{\sigma,i+1}) + U \sum_i n_{\uparrow,i} n_{\downarrow,i} + V \sum_i n_i n_{i+1}.$$



M. Tsuchiizu, PRL (2002)

$$\mathcal{O}_{\mathrm{CDW}} \equiv (-1)^j n_j$$

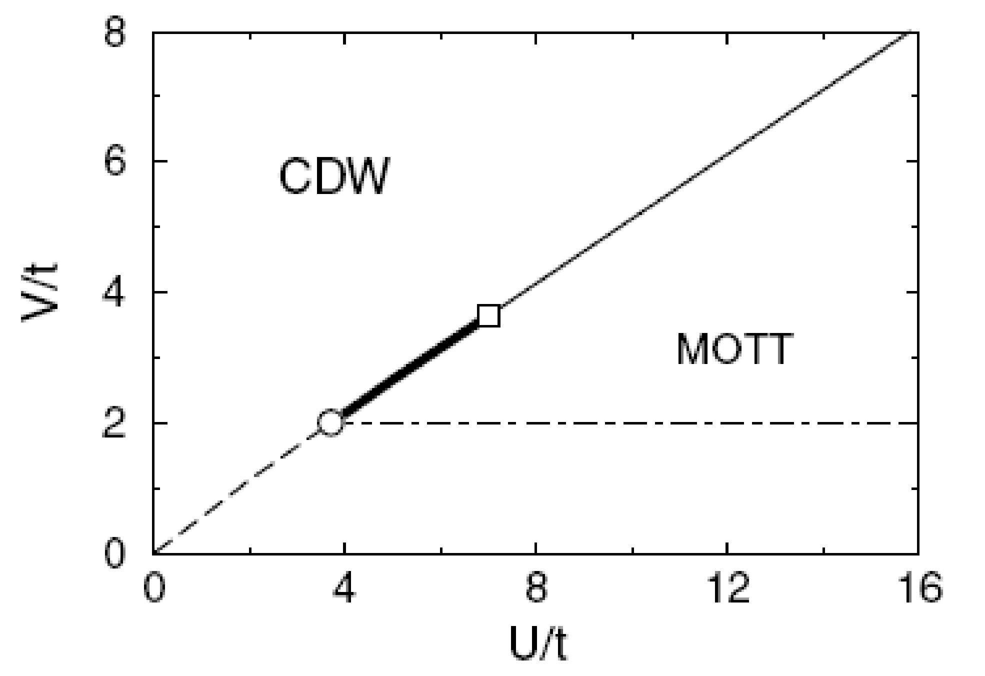
$$\mathcal{O}_{\mathrm{SDW}} \equiv (-1)^j (n_{j,\uparrow} - n_{j,\downarrow})$$

$$\mathcal{O}_{\mathrm{BCDW}} \equiv (-1)^j \sum_\sigma (c^\dagger_{j,\sigma} c_{j+1,\sigma} + \mathrm{H.c.})$$

Extended Hubbard Model

At Half-filling

$$H = -t \sum_{\sigma=\uparrow,\downarrow} \sum_i (c^\dagger_{\sigma,i+1} c_{\sigma,i} + c^\dagger_{\sigma,i} c_{\sigma,i+1}) + U \sum_i n_{\uparrow,i} n_{\downarrow,i} + V \sum_i n_i n_{i+1}.$$

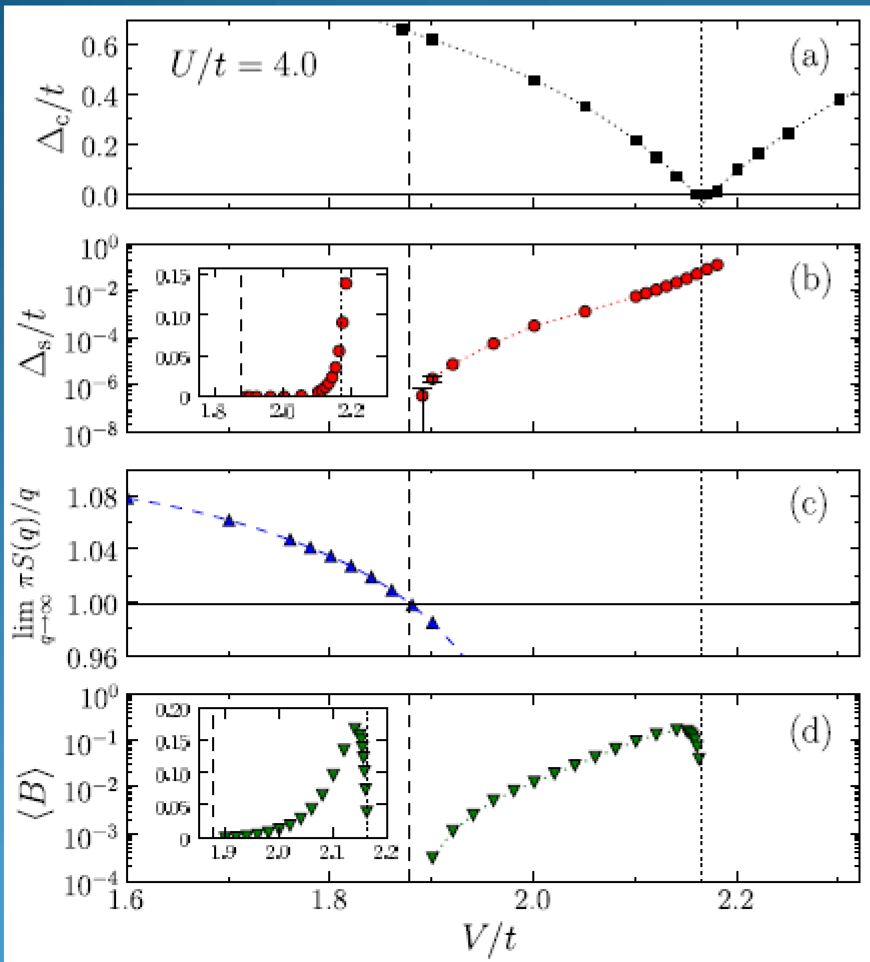


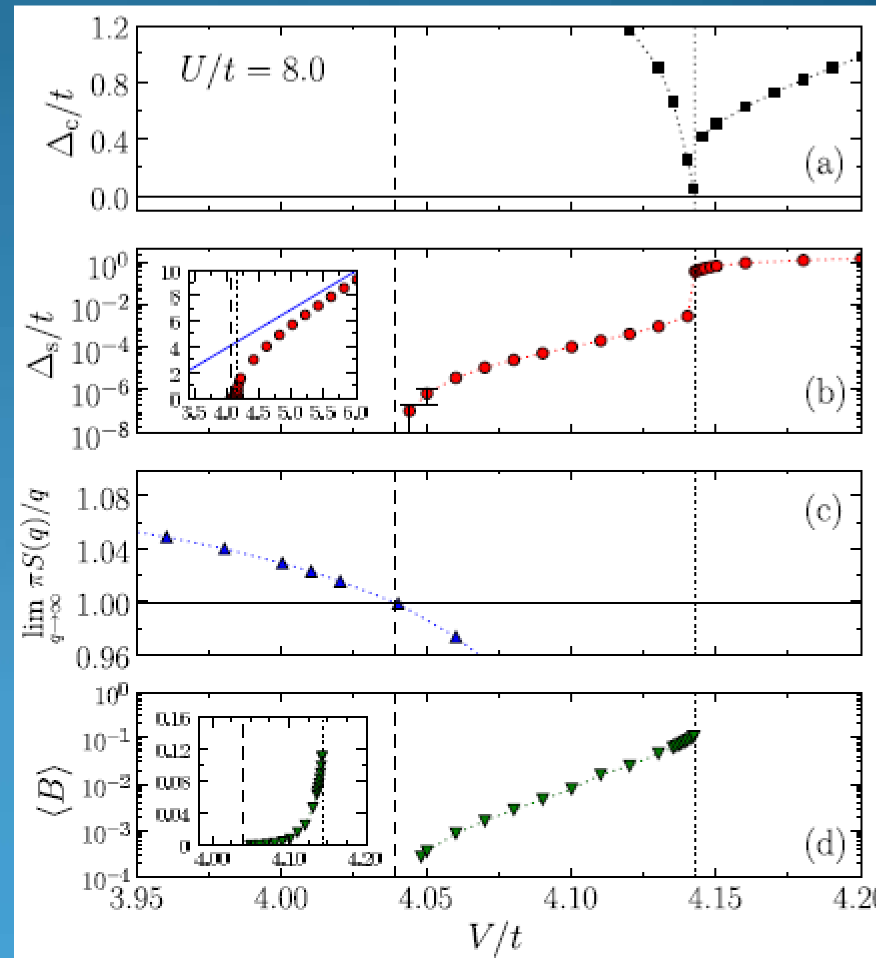
E. Jeckelmann, PRL (2002)

Extended Hubbard Model

At Half-filling

$$K_{\rho,\sigma} = \frac{1}{\pi q} S_{\rho,\sigma}(q \to 0).$$

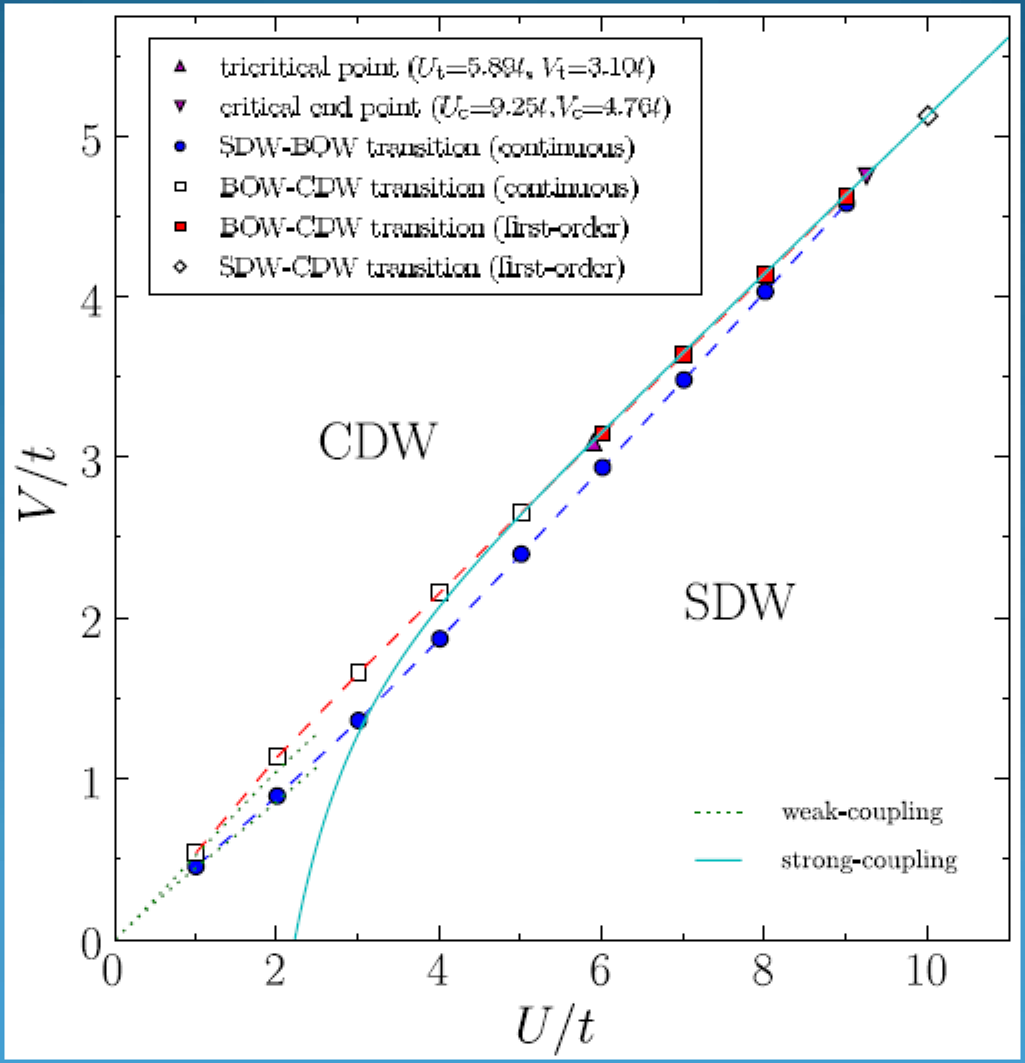




S. Ejima, PRL (2002)

Extended Hubbard Model

At Half-filling



A.W. Sandvik, PRL (2004)
S. Ejima, PRL (2007)

Extended Hubbard Model

At quad-filling

The charge gap

$$\Delta(L;N) = E_0(L;N+1) + E_0(L;N-1) - 2E_0(L;N).$$

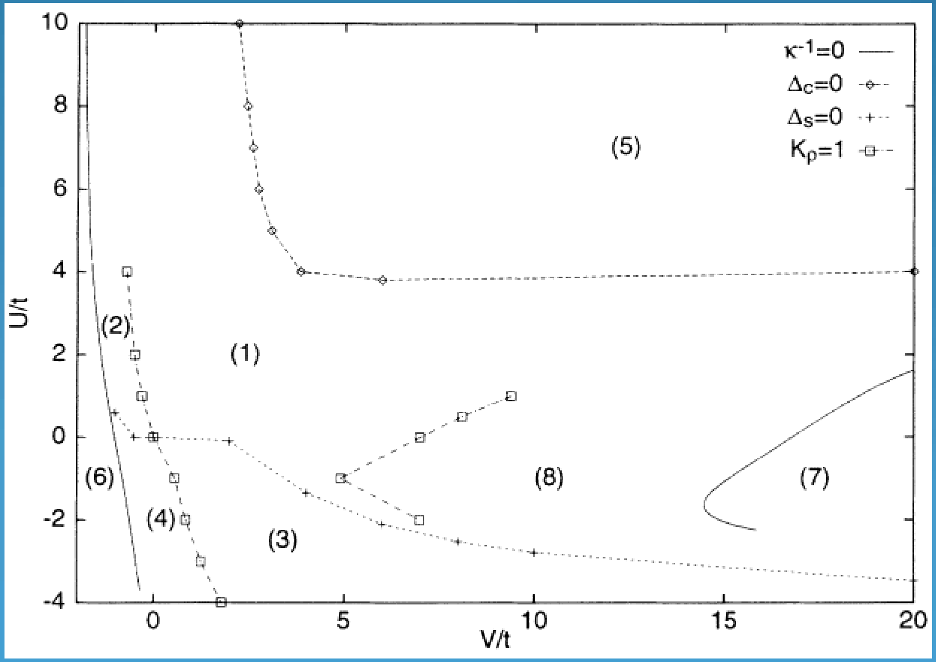
The spin gap

$$\Delta_s(L;N) = E_0(L;N;S^z=1) - E_0(L;N;S^z=0).$$

The compressibility

$$\kappa = \frac{L}{N^2}\left(\frac{E_0(L;N+2) + E_0(L;N-2) - 2E_0(L;N)}{4}\right)^{-1}.$$

1. SDF
2. SSF
3. CDF
4. SSF
5. SDW
6. PS
7. PS
8. TSF



K. Penc, PRB (1994)

The next session

- Hubbard model with additional terms
- Metal-insulator transition
- Nonlocal long range order
- Phase diagram of polarized state
- The effect of long-range interaction
- The phase diagram of dipolar fermions

Tomorrow ; 14:30-15:30