# *Overview for Models and Methods of Strongly Correlated Systems*

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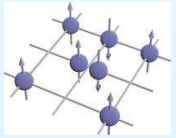

# Outline

- Strongly correlated electrons
  - 3D systems
  - Low-dimensional systems
- Models
  - The Hubbard model and its extensions
  - Impurity models
- Methods
  - Numerical methods
  - Analytical methods
- An example: the $t$-$U$-$J_1$-$J_2$ model

# Strongly correlated electrons - General features

Treating the electronic correlations:

- In general by Hartree–Fock approximation (single-particle picture).
  - Hartree term - interaction with a homogenous background.
  - Fock term - correction to the Hartree approximation by an exchange term.
- Beyond the Hartree–Fock theory - correlation effects.
  - $E_{corr}/E_{HF}$ is large enough $\longrightarrow$ strong correlation.
- Large effective mass (beyond the single-particle picture) $\longrightarrow$ strong correlation.
- Qualitatively incorrect result by the HF approximation $\longrightarrow$ strong correlation.

In strongly correlated systems:

- Single-particle picture fails.
- Competing energy scales: itinerant or localised electrons?

# Strongly correlated electrons - 3D systems

Transition and rare earth metal compounds:

$d$- and $f$-electron systems.

Electronic properties:

Conduction band and narrow $d$- or $f$-band.

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- Mixed valence systems $\rightarrow$

Simple case: single impurity ion with partly filled $f$-orbital in an $s$-band metal.

The energy levels: $\epsilon_f^{(n)}$

Hybridization $\rightarrow \epsilon_f^{(n=l)}$ is close to $E_{Fermi}$.

Allowed configurations: $4f^l$ and $4f^{l-1} \rightarrow$ fluctuating or noninteger valence.

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- Mixed valence systems
- Heavy fermion systems

$\rightarrow$

Special mixed valence system: the dominating allowed configuraton has magnetic moment.

Linear $T$-dependence of the specific heat,

$T$-independent Pauli-susceptibility with unusual large coefficient $\rightarrow$ „normal” metal, but

Hybridization leads to $m^*$ up to $\mathcal{O}(1000 m_0)$.

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Behind the pairing mechanism stands

- e-ph interaction in conventional SCs.

- electron correlation (e-e interaction) in HTSCs.

Highly anisotrop materials.

2D models for HTSC: fluctuating valence (Cu $d^8$-$d^9$ or $d^9$-$d^{10}$), heavy $d$-electron systems (Cu $d^9$).

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- Mixed valence systems
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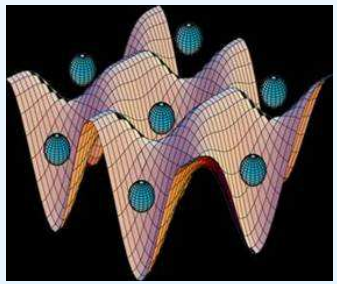
- High $T_c$ superconductors
- (Ultracold fermions)

$\rightarrow$

To simulate condensed matter phenomenas:

- Ideal lattice (no distorsion, impurity, etc.),
- Well controllable parameters



# Strongly correlated electrons - Low-dimensional systems

One-dimensional systems:

- Highly anisotropic materials, nanotubes, organic conductors, quantum wires (confined electrons to a line), etc.
- A number of exotic phases: spin-, and charge-density waves, superconductivity, non-Fermi liquid state, etc.

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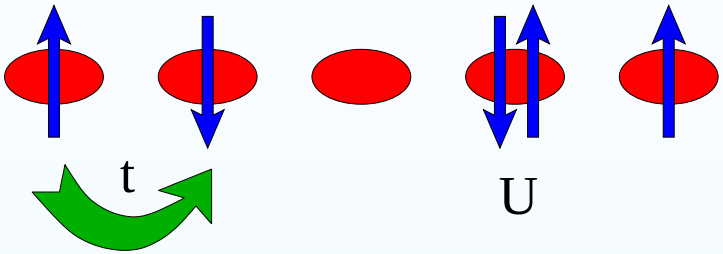
Zero-dimensional systems: quantum dots - confined electrons to a point.

- Multiple quantum dots, quantum dot lattices (electrode grid, embeddig QDs into an organic medium, etc.).
- Well controllable properties: size, shape, number of electrons, transparency of the confining barriers, etc. $\rightarrow$ testing of fundamental quantum mechanical problems, e.g exact 1D crystal with PBC: pearl-necklace-like quantum dot string [Kouwenhoven, Delft Univerity].

# Models - Hubbard model and its extensions

- Nearest-neighbor hopping $t$.
- On-site Coulomb interaction $U$.




The Hamiltonian of the Hubbard model:

$$\mathcal{H}_{t\text{-}U} = t \sum_{\langle i,j \rangle, \sigma} c^{\dagger}_{i,\sigma} c_{j,\sigma} + \frac{U}{2} \sum_{\sigma \neq \sigma'} \sum_{i} n_{i,\sigma} n_{i,\sigma'}.$$

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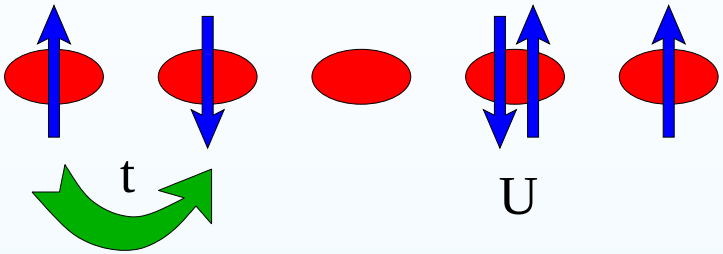


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e.g. Mott-transition, para-, ferro-, and antiferromagnetic phases (2D, J. E. Hirsch, 1985), spiral SDW, special ferrimagnetic states (3D, D. R. Penn, 1966), $d$-SC.

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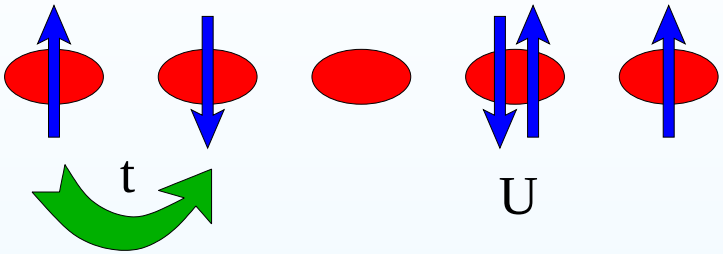


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For $d$-electrons: $U \sim 20$ eV, nearest-neighbor repulsion $V \sim 6$ eV (screening: 2-3 eV).

The Hamiltonian of the extended Hubbard model:

$$\mathcal{H} = t \sum_{\langle i,j \rangle, \sigma} c^{\dagger}_{i,\sigma} c_{j,\sigma} + \frac{U}{2} \sum_{\sigma \neq \sigma'} \sum_{i} n_{i,\sigma} n_{i,\sigma'} + \frac{V}{2} \sum_{\sigma,\sigma'} \sum_{\langle i,j \rangle} n_{i,\sigma} n_{j,\sigma'}.$$

# Models - Hubbard model and its extensions

Numerous extensions for different limits and depending on the studied phenomena.

- Role of exchange interaction: $\mathcal{H} = \mathcal{H}_{t\text{-}U} + J \sum_{\langle i,j \rangle} \mathbf{S}_i \mathbf{S}_j .$

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- Role of the magnetic frustration: $\mathcal{H} = \mathcal{H}_{t\text{-}U} + J \sum_{\langle i,j \rangle} \mathbf{S}_i \mathbf{S}_j + J' \sum_{[i,j]} \mathbf{S}_i \mathbf{S}_j .$

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- Strong repulsion ($n \neq 1$): $\mathcal{H} = t \sum_{\langle i,j \rangle, \sigma} c^{\dagger}_{i,\sigma} c_{j,\sigma} + J \sum_{\langle i,j \rangle} \mathbf{S}_i \mathbf{S}_j .$

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- Long(er)-range-hopping: $\mathcal{H} = \sum_{i,j,\sigma} t_{i,j} c^{\dagger}_{i,\sigma} c_{j,\sigma} + \frac{U}{2} \sum_{\sigma \neq \sigma'} \sum_i n_{i,\sigma} n_{i,\sigma'} .$

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- Orbital degenaration/multiband systems:

  $\mathcal{H} = t \sum_{\langle i,j \rangle, \mu, \nu, \sigma} c^{\dagger}_{i,\mu,\sigma} c_{j,\nu,\sigma} + \frac{U}{2} \sum_{\mu,\nu,\sigma,\sigma'} \sum_i n_{i,\mu,\sigma} n_{i,\nu,\sigma'} .$

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- Multicomponent fermions: $\mathcal{H} = \mathcal{H}_{t\text{-}U}$ with $\sigma = 1, 2, \ldots, f .$

# Models - Imurity models - Anderson model

Applications: Magnetic impurities in normal metals, transport properties of QDs.

Simple example: single non-degenerate $d$-, or $f$-type impurity (ion) in an $s$ electron system $\longrightarrow$ The non-degenerate single impurity Anderson model:

$$\mathcal{H} = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} + \sum_{\sigma} \epsilon_d d^{\dagger}_{\sigma} d_{\sigma} + U n^{(d)}_{\uparrow} n^{(d)}_{\downarrow} + \frac{1}{\sqrt{V}} \sum_{\mathbf{k},\sigma} \left( V_{d\mathbf{k}} c^{\dagger}_{\mathbf{k},\sigma} d_{\sigma} + V_{\mathbf{k}d} d^{\dagger}_{\sigma} c_{\mathbf{k},\sigma} \right).$$

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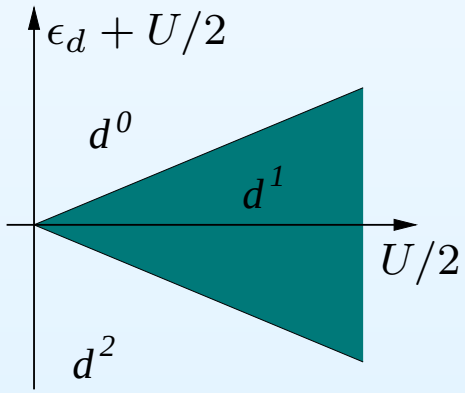
Formation of a magnetic moment:

- Without hybridization:
  - Energy levels of the ion:

    $\epsilon(d^0) = 0$, $\epsilon(d^1) = \epsilon_d$, $\epsilon(d^2) = 2\epsilon_d + U$.
  - Requirements for finite magnetic moment:

    $\epsilon(d^0) > \epsilon(d^1)$ and $\epsilon(d^2) > \epsilon(d^1)$.



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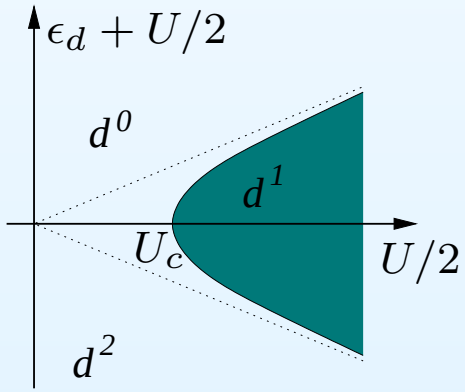
Formation of a magnetic moment:

- With hybridization (mean-field approximation):
  - Resonance peak at $\epsilon_d + U\langle n^{(d)}_{-\sigma} \rangle$ with FWHM $\Delta$.
  - $\pi \langle n^{(d)}_{-\sigma} \rangle = \mathrm{ctg}^{-1} \left[ (\epsilon_d + U\langle n^{(d)}_{-\sigma} \rangle)/\Delta \right]$.
  - For $U < U_c$: $\langle n^{(d)}_{\sigma} \rangle = \langle n^{(d)}_{-\sigma} \rangle = n_d/2$.
  - For $U > U_c$: $\langle n^{(d)}_{\sigma} \rangle = n_d/2 + \sigma \delta n_d$.



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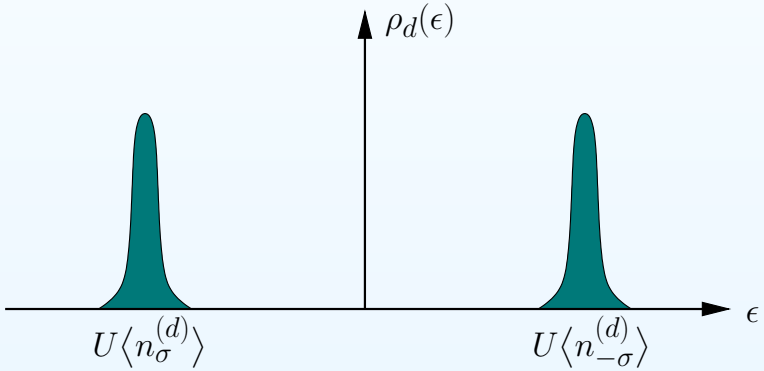
Kondo regime: $\epsilon_d + U\langle n_\sigma^{(d)}\rangle < E_{Fermi} < \epsilon_d + U\langle n_{-\sigma}^{(d)}\rangle$.

Mean-field approximation:



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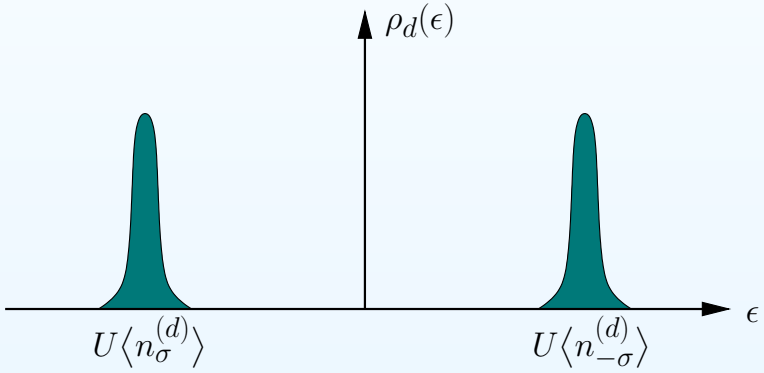
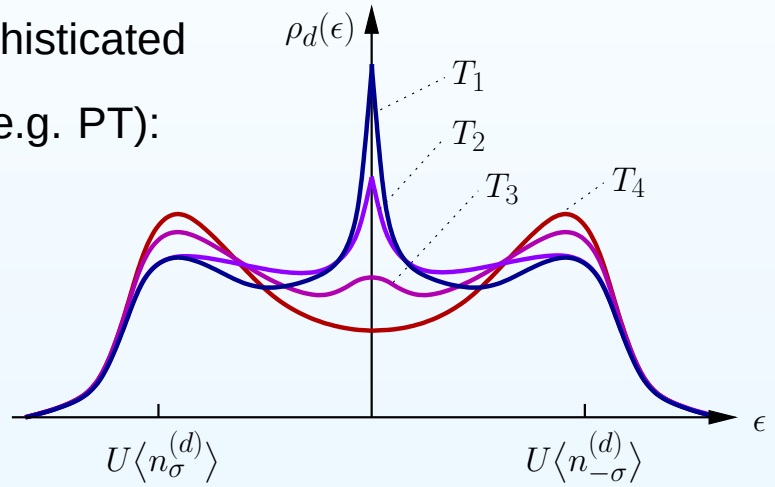



More sophisticated methods (e.g. PT):




Kondo (Abrikosov-Suhl) resonance

$T_1 < T_2 < T_3 < T_4$

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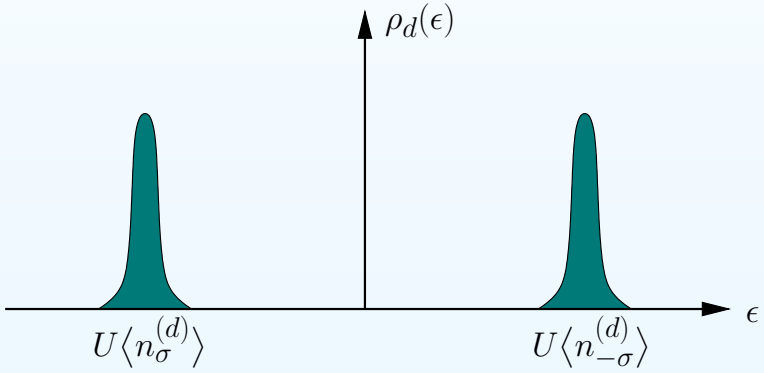


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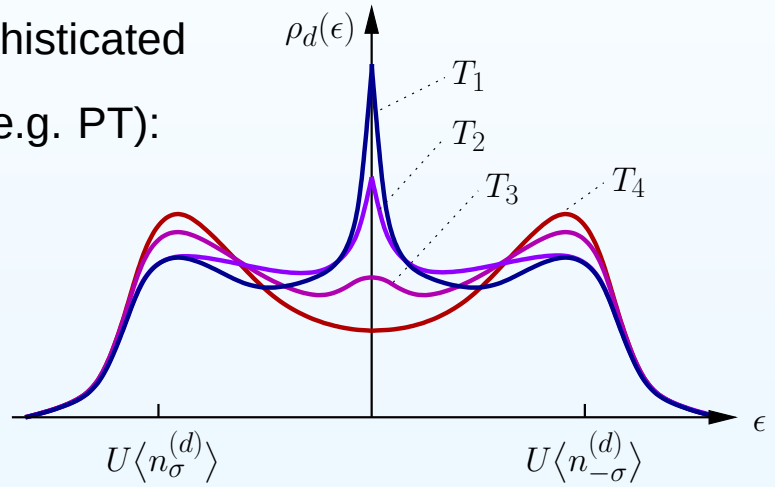


Kondo (Abrikosov-Suhl) resonance

$T_1 < T_2 < T_3 < T_4$

- Localized magnetic moment as scattering potential.
- Higher T: free magnetic moment - Curie susceptibility.
- Lower T: strong correlation with the conduction electrons - Kondo problem.

# Models - Impurity models - Kondo model

Studying the effect of the localized magnetic moment:

- Allowed configurations: $d^\sigma$ - no charge fluctuation (Kondo regime).
- Canonical transformation: Anderson model $\longrightarrow$ $s$-$d$ exchange model.

$$\mathcal{H}_{s\text{-}d} = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} - \frac{1}{V} \sum_{\mathbf{k},\mathbf{k}',\sigma,\sigma'} J_{\mathbf{k},\mathbf{k}'} \mathbf{S} \cdot \sigma_{\sigma,\sigma'} c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k}',\sigma'}$$

Antiferromagnetic exchange if $J_{\mathbf{k},\mathbf{k}'} < 0$.

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Antiferromagnetic exchange if $J_{\mathbf{k},\mathbf{k}'} < 0$.

- $|\epsilon_{\mathbf{k}}|, |\epsilon_{\mathbf{k}'}| \ll |\epsilon_d + U\langle n^{(d)}_\sigma \rangle|$ for $\sigma = \uparrow, \downarrow$.
- In the restricted Hilbert space and $J_{\mathbf{k},\mathbf{k}'} =$ const. $\rightarrow$ Kondo model (J>0):

$$\mathcal{H}^K_{int} = \frac{J}{V} \sum_{\mathbf{k},\mathbf{k}'} \left[ S^+ c^\dagger_{\mathbf{k},\uparrow} c_{\mathbf{k}',\downarrow} + S^- c^\dagger_{\mathbf{k},\downarrow} c_{\mathbf{k}',\uparrow} + S^z (c^\dagger_{\mathbf{k},\uparrow} c_{\mathbf{k}',\uparrow} - c^\dagger_{\mathbf{k},\downarrow} c_{\mathbf{k}',\downarrow}) \right]$$

- IR divergency at $E_{Fermi}$ at $T = 0$ in leading order - the PT fails.
- New methodes: RG treatment, scaling theory.

# Models - Impurity models - Multiple impurities

Applications: mixed valence systems, heavy fermions, QD-islands, QD-lattices, QD-arrays etc.

- Interesting regime: $\epsilon_f + U\langle n_\sigma^{(f)}\rangle \approx E_{Fermi}$ - charge fluctuation.

$$\mathcal{H} = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} + \sum_{i,\sigma} [\epsilon_f f^\dagger_{i,\sigma} f_{i,\sigma} + U n^{(f)}_{i,\uparrow} n^{(f)}_{i,\downarrow}] + \mathcal{H}_{hyb}$$

  - Periodic Anderson model:

$$\mathcal{H}_{hyb} = \frac{1}{\sqrt{V}} \sum_{i,\mathbf{k},\sigma} \left( V_{\mathbf{k}} \mathrm{e}^{i\mathbf{k}\mathbf{R}_i} c^\dagger_{\mathbf{k},\sigma} f_{i,\sigma} + V^*_{\mathbf{k}} \mathrm{e}^{-i\mathbf{k}\mathbf{R}_i} f^\dagger_{i,\sigma} c_{\mathbf{k},\sigma} \right).$$

  - Multiple impurity Anderson model:

$$\mathcal{H}_{hyb} = \frac{1}{\sqrt{V}} \sum_{i,\mathbf{k},\sigma} \left( V_{\mathbf{k}} c^\dagger_{\mathbf{k},\sigma} f_{i,\sigma} + V^*_{\mathbf{k}} f^\dagger_{i,\sigma} c_{\mathbf{k},\sigma} \right).$$

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  - Periodic Anderson model:

$$\mathcal{H}_{hyb} = \frac{1}{\sqrt{V}} \sum_{i,\mathbf{k},\sigma} \left( V_{\mathbf{k}} \mathrm{e}^{i\mathbf{k}\mathbf{R}_i} c^\dagger_{\mathbf{k},\sigma} f_{i,\sigma} + V^*_{\mathbf{k}} \mathrm{e}^{-i\mathbf{k}\mathbf{R}_i} f^\dagger_{i,\sigma} c_{\mathbf{k},\sigma} \right).$$

  - Multiple impurity Anderson model:

$$\mathcal{H}_{hyb} = \frac{1}{\sqrt{V}} \sum_{i,\mathbf{k},\sigma} \left( V_{\mathbf{k}} c^\dagger_{\mathbf{k},\sigma} f_{i,\sigma} + V^*_{\mathbf{k}} f^\dagger_{i,\sigma} c_{\mathbf{k},\sigma} \right).$$

- Kondo regime: $\epsilon_f + U\langle n_\sigma^{(f)}\rangle < E_{Fermi} < \epsilon_f + U\langle n_{-\sigma}^{(f)}\rangle$ - Kondo lattice.

$$\mathcal{H} = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} + \frac{J}{V} \sum_{i,\mathbf{k},\mathbf{k}',\sigma,\sigma'} \mathrm{e}^{-i(\mathbf{k}-\mathbf{k}')\mathbf{R}_i} \, \mathbf{S}_i \cdot \sigma_{\sigma,\sigma'} c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k}',\sigma}$$

# Methods - Numerical methods

## Dynamical mean-field theory (DMFT):

Aim: to approximate a many-particle problem by an effective single-particle problem.

E.g. Ising model:

$$\mathcal{H} = -\sum_{(i,j)} J_{ij} S_i S_j - h \sum_i S_i$$

$$\mathcal{H}_{eff} = -\sum_i h_i^{eff} S_i.$$

Effective Weiss field: $h_{eff}$

Mean-field approximation:

$$\langle S_i S_j \rangle \approx \langle S_i \rangle \langle S_j \rangle.$$

Self-consistency relation:

$$\langle S_i \rangle_{\mathcal{H}_{eff}} \stackrel{!}{=} \langle S_i \rangle$$

DMFT for the Hubbard model:

$$\mathcal{H} = -\sum_{i,j,\sigma} t_{ij} c_{i,\sigma}^\dagger c_{j,\sigma} + U \sum_i n_{i,\uparrow} n_{i,\downarrow} + \epsilon_0 \sum_{i,\sigma} n_{i,\sigma}$$

$$\mathcal{H}_{eff} = \mathcal{H}_{SIAM}, \quad \mathcal{H}_{bath} = \sum_{k,\sigma} \varepsilon_k b_{k,\sigma}^\dagger b_{k,\sigma}$$

$$\mathcal{H}_{atom} = U n_\uparrow^{(a)} n_\downarrow^{(a)} + (\epsilon_0 - \mu)(n_\uparrow^{(a)} + n_\downarrow^{(a)})$$

$$\mathcal{H}_{coupling} = \sum_{k,\sigma} V_k (b_{k,\sigma}^\dagger a_\sigma + a_\sigma^\dagger b_{k,\sigma})$$

Effective Weiss function: $\Delta(E) = \sum_k \frac{|V_k|^2}{E - \varepsilon_k}$

Mean-field approximation:

The self-energies: $\Sigma_{ii} \approx \Sigma_{imp}$, $\Sigma_{i \neq j} \approx 0$.

Self-consistency relation:

The Green's functions: $G_{ii} \stackrel{!}{=} G_{imp}$.

# Methods - Numerical methods

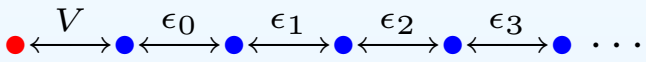
Numerical renormalization group: Applications: impurity models.

$$\mathcal{H} = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} + \mathcal{H}_{imp}[d, d^{\dagger}] + \sum_{\mathbf{k},\sigma} V \left( c^{\dagger}_{\mathbf{k},\sigma} d_{\sigma} + d^{\dagger}_{\sigma} c_{\mathbf{k},\sigma} \right).$$

- Logarithmic discretization of the DOS of the $c$ electrons (interval - single state).
- This discrete model is mapped on a semi-infinite lattice-like model

$$\tilde{\mathcal{H}} = \sum_{\sigma} \sum_{n=0}^{\infty} \epsilon_n c^{\dagger}_{n,\sigma} c_{n,\sigma} + \mathcal{H}_{imp}[d, d^{\dagger}] + \sum_{\sigma} V \left( c^{\dagger}_{0,\sigma} d_{\sigma} + d^{\dagger}_{\sigma} c_{0,\sigma} \right).$$

  Hopping decreases exp. along the chain:




- RG treatment:
  - The lattice constructed site-by-site.
  - Truncation procedure: ∼100 lowest energy eigenstates.
- $N \to \infty$: fixed point behavior.

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  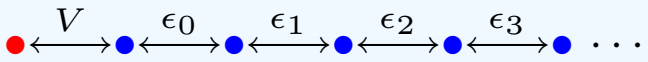
  

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Density-matrix renormalization group: Application: 1D lattice models (spin, fermion, boson).

- Construction of the full system by a series of subsystem with increasing size.
- A part of the system is handled as environment.
- Systematic truncation of the Hilbert space - keeping the most probable eigenstates of the reduced density-matrix.

# Methods - Analytical methods

Gutzwiller ansatz (for the Hubbard model):

- $U = 0$: fluctuation of the local polarization - deviation from the local charge neutrality.
- $U \neq 0$: minimal polarization (Van Vleck, 1953).

$$|FS\rangle = \prod_{\mathbf{k}} c^{\dagger}_{\mathbf{k},\uparrow} \prod_{\mathbf{k}'} c^{\dagger}_{\mathbf{k}',\downarrow} |0\rangle = \frac{1}{L^N} \sum_{\{i\uparrow\}} \sum_{\{j\downarrow\}} F(\{i\uparrow\}) F(\{j\downarrow\}) \prod_{i} c^{\dagger}_{i,\uparrow} \prod_{j} c^{\dagger}_{j,\downarrow} |0\rangle$$

- In the uncorrelated metallic phase every localized configuration appear.
- $F(\{i\uparrow\})$, $F(\{j\downarrow\})$ are independent ($|FS\rangle$ is uncorrelated) - double occupied sites.
- The projection of these states: $|\Psi_G\rangle = \eta^D |FS\rangle = \prod_i \left[1 - (1-\eta) n_{i\uparrow} n_{j\downarrow}\right] |FS\rangle$

  $g < 1$ and $D = \sum_i n_{i\uparrow} n_{i\downarrow}$.
- Treating the determinants $F(\{i\uparrow\})$, $F(\{i\downarrow\}) \rightarrow$ Gutzwiller approximation.
- Minimalization of the energy functional:

$$E_0 = \frac{\langle \Psi_G | H | \Psi_G \rangle}{\langle \Psi_G | \Psi_G \rangle}.$$

# Methods - Analytical methods

Renormalization group (RG) treatment in solid state physics:

Applications: - long wavelength behavior (e.g. critical phenomena, Kondo model),

- low energy behavior (e.g. 1D electron systems)

of scale invariant systems.

Iteration: integrating out of the short distance/high energy degrees of freedom.

$$F[\{g_i\}] \longrightarrow g_i \to \tilde{g}_i \longrightarrow \tilde{F}[\{\tilde{g}_i\}]$$

Fixed point behavior: relevant, irrelevant, marginal operators.

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## Slave-boson method:

Interacting fermion system: $H[c, c^\dagger] \to$ Partition function: $Z = \int [\mathrm{d}c][\mathrm{d}c^\dagger] \exp(-S[c, c^\dagger])$

HS fields - generally fluctuating charge ($\phi$) and spin ($\chi$) densities.

$$Z = \int [\mathrm{d}\phi][\mathrm{d}\chi][\mathrm{d}c][\mathrm{d}c^\dagger] \exp(-S[c, c^\dagger; \phi, \chi]) = \int [\mathrm{d}\phi][\mathrm{d}\chi] \exp(-\tilde{S}_{\mathrm{eff}}[\phi, \chi])$$

Saddle-point approximation $\to$ dominant HS fields - relevant bosonic configurations

Slave bosons

# Methods - Analytical methods

Bosonization:

One of the most powerful nonperturbative technique for 1D fermion systems.

Aim: transform the complicated interacting model into an equivalent weakly interacting one.

- Absence of the Fermi surface (and quasiparticles) $\rightarrow$ density fluctuations.

- Boson-like particle-hole pair excitations ($v_e \approx v_h$) $\rightarrow$ propagating collective modes.

- One particle operator can also be expressed by boson operators!

$\Psi_\sigma \sim F(\Phi_\sigma) \quad \longrightarrow \quad \mathcal{H}_f[\Psi_\sigma] \rightarrow \mathcal{H}_b[\Phi_\sigma]$ , $\quad F(\Phi_\sigma)$ nonlinear, nonlocal.

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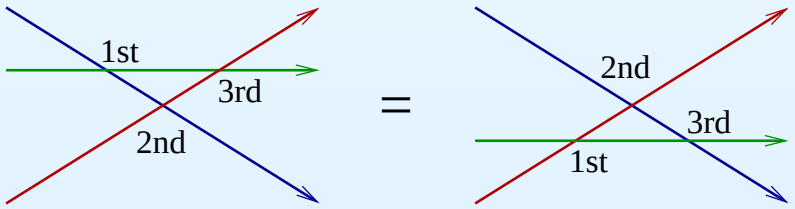
Bethe ansatz: Application: exactly solvable 1D systems - completely integrable:

No. of degrees of freedom $=$ No. of conserved quantities.

Multiparticle scattering processes as the series of two-particle scatterings and these processes statisfy the Yang-Baxter equation:



# An example: the $t$-$U$-$J_1$-$J_2$ model

The Hamiltonian:

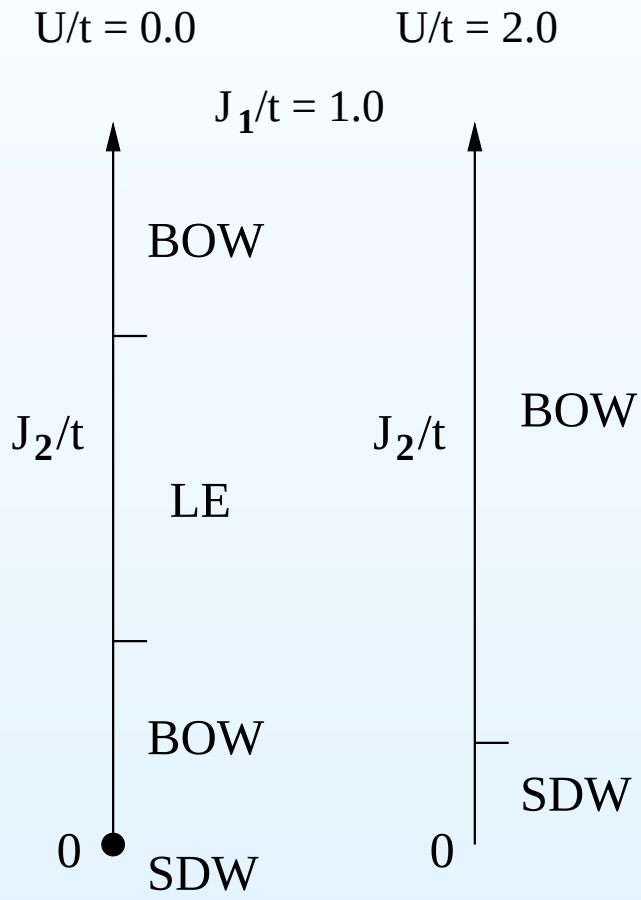
$$\mathcal{H} = t \sum_{\langle i,j \rangle, \sigma} c^{\dagger}_{i,\sigma} c_{j,\sigma} + \frac{U}{2} \sum_{\sigma \neq \sigma'} \sum_{i} n_{i,\sigma} n_{i,\sigma'} + J \sum_{\langle i,j \rangle} \mathbf{S}_i \mathbf{S}_j + J' \sum_{[i,j]} \mathbf{S}_i \mathbf{S}_j$$

The ground state phase diagram of the 1D model was investigated

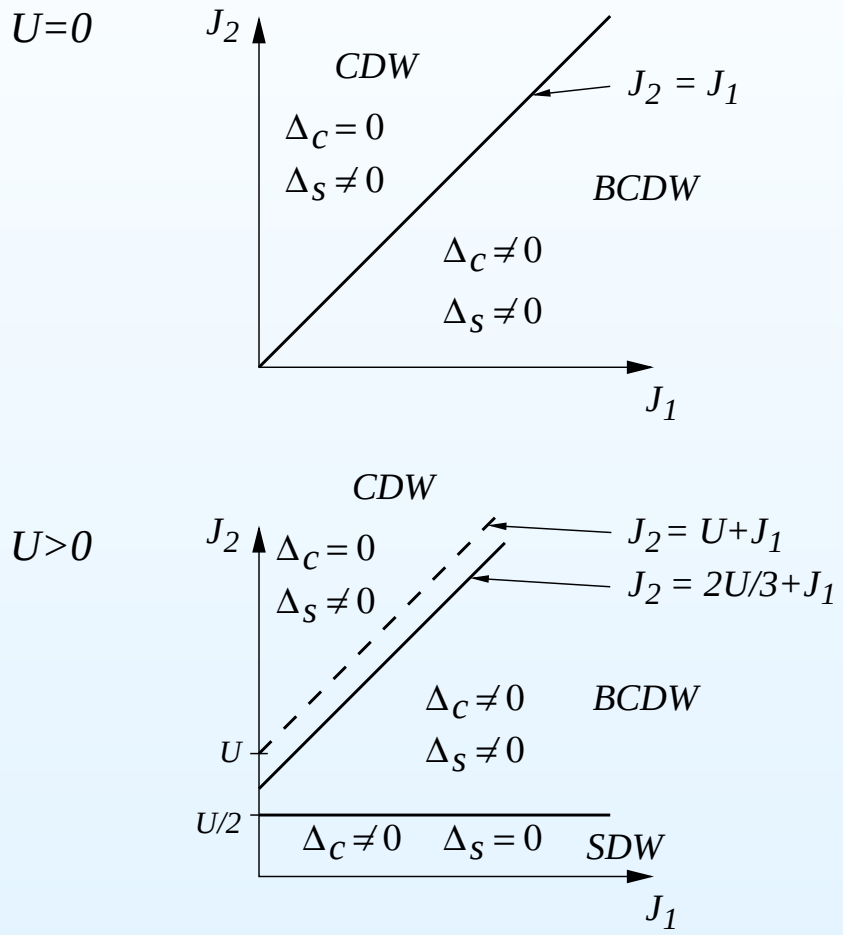
- numerically by real-space DMRG method (spin gap, charge gap, staggered bond order parameter).
- analytically by bosonization of the $g$-ology Hamiltonian combined with RG treatment and semiclassical analysis (charge gap, spin gap, dominant correlations).

# An example: the $t$-$U$-$J_1$-$J_2$ model

Numerical results:




Analytical results:



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*Thank you for your attention*.