Order and Transport in Complex Quantum Systems: Pars non pro toto

Holger Fehske

Universität Greifswald

Problem: highly correlated systems $\neq \sum$ weakly interacting parts

" the whole is greater than its parts"

. . . quasi-1D metals & quantum spin systems, . . .

. . . high-T_c cuprates, CMR manganites, heavy fermion materials, . . .

. . . novel semiconductors, . . . , complex plasmas, . . .

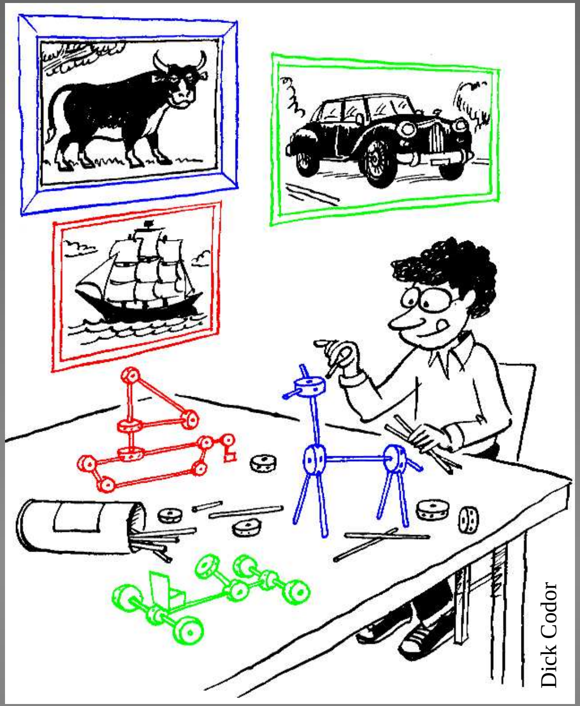
Preface

How to proceed?

physical system

“microscopic” ↓ approach

construction of minimal models



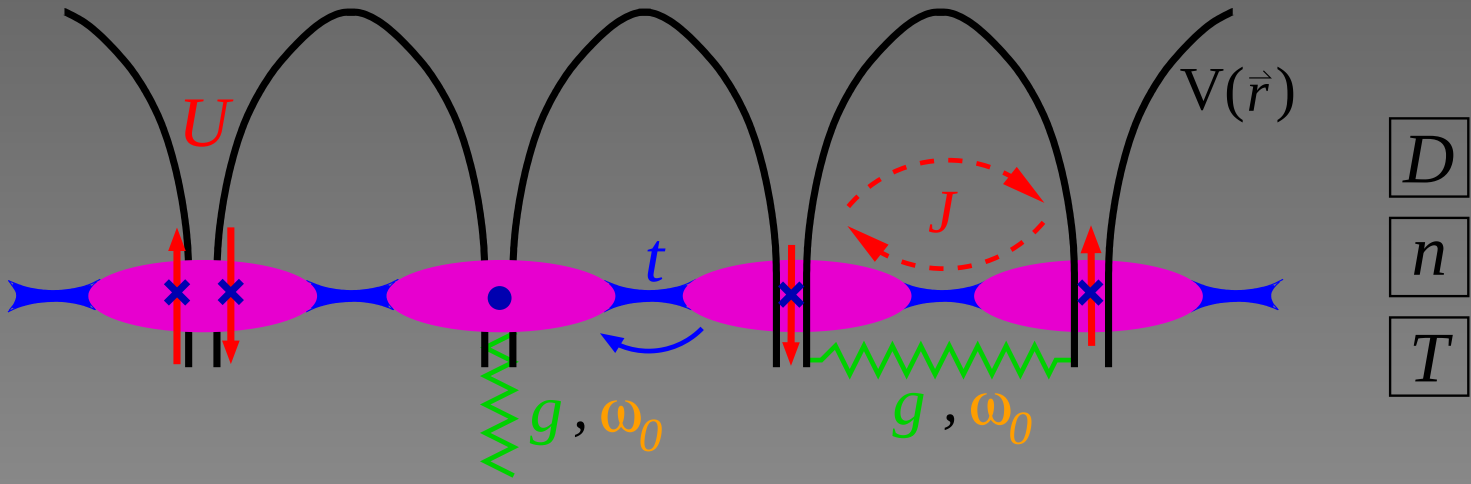
Hamiltonian

reliable theory | and numerics

ground state properties	thermodynamics, excitation spectra	dynamical correlation functions
E_0, $\|\psi_0\rangle$, $\langle ... \rangle_0$	E_n, Z, c_v, $\ldots$	$\sigma(\omega)$, $\chi(q,\omega)$, $\ldots$

$\longrightarrow$ comparison with experiment

Indication of ingredients



$\rightsquigarrow$ Complex interplay of charge, spin, orbital, and lattice degrees of freedom !

▶ Minimal models? ... **Holstein-Hubbard Hamiltonian:**

$$H = \sum_i \epsilon_i n_{i\sigma} - t \sum_{\langle i,j \rangle} c_{i\sigma}^{\dagger} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} - g\,\omega_0 \sum_{i\sigma} (b_i^{\dagger} + b_i) n_{i\sigma} + \omega_0 \sum_i b_i^{\dagger} b_i$$

✗ Problem: not solvable even in 1D (also not for just one e$^-$ or at $n = 1$)!

✗ Approximations? Bad luck! “Standard” many-body techniques fail in most interesting cases... ☹

Outline

Way out? Exact numerical study of finite systems (+ finite-size scaling...)!

I. Sketch of selective numerical approaches

Hager, Wellein (Erlangen), Jeckelmann (Mainz), Schubert (Greifswald), Weiße (Sydney)

II. Anderson localisation & quantum percolation

Disordered electron systems

Alvermann, Bronold, Schubert (Greifswald)

III. Quantum phase transitions in 1D

Luttinger liquids

Peierls & Mott insulators

Bishop (LANL), Becker (Dresden), Kampf (Augsburg)

IV. Charge-spin-orbital-lattice coupling effects

CMR manganites

Loos (Prague), Weiße (Sydney)

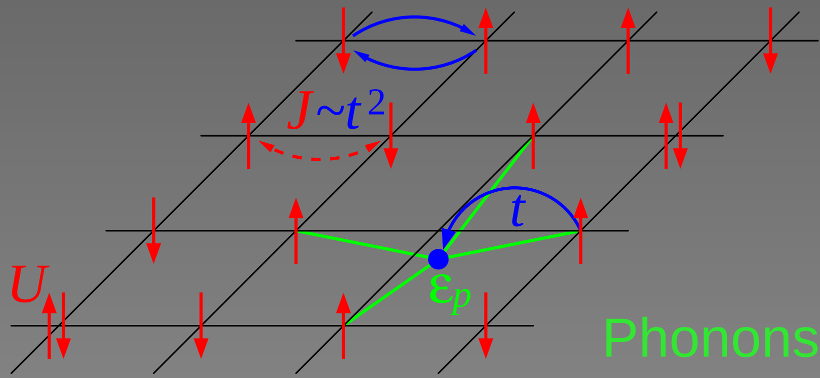
V. Bound state formation & Wigner crystallisation

Electon-hole plasmas

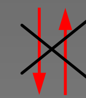
Bonitz (Kiel), Filinov (Moscow)

Focus: Interplay of order & transport phenomena!

I. 1. Exact treatment of finite quantum systems



Fermions: 4^N (Hubbard)


$\rightarrow$ 3^N (t-J-model)

$n=1$ $\rightarrow$ 2^N (Heisenberg)

Phonons: $D_p = \infty$ even for 1e$^-$ $\Rightarrow$ truncation of H ($\rightsquigarrow \tilde{M}$)!?

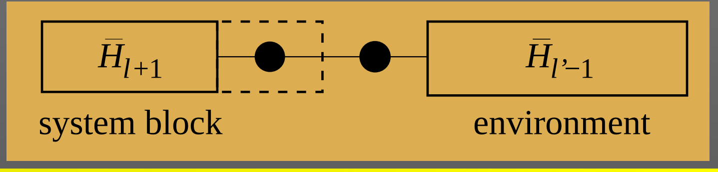
Basis optimisation: $|\psi\rangle = \sum_{e,p} C_{ep}^{\psi} \{|e\rangle \otimes |p\rangle\}$ $\rightarrow$ $|\tilde{p}\rangle = \sum_{p}^{D_p} \alpha_{\tilde{p}p} |p\rangle$ $(D_{\tilde{p}} < D_p)$

minimize $\left\| |\psi\rangle - |\tilde{\psi}\rangle \right\|^2$ $(\propto 1 - \mathrm{Tr}\{\alpha\rho\alpha^\dagger\})$ w. r. t. α (density matrix algorithm)

$\Rightarrow$ **Eigenvalue problem of large sparse Hermitian matrices**

Ground-state properties:

- Lanczos (ED) method: $H^D \rightarrow T^L$, $(L \ll D)$, $D \lesssim 10^{11}$, E_0, $|\psi_0\rangle$
- Jacobi Davidson algorithm: E_n, $|\psi_n\rangle$, $n \lesssim 30$, $D \lesssim 10^7$, $N = 8\ldots36$
- Density Matrix Renormalisation Group: $N = 128\ldots512$



I. 2. KPM & MEM

Spectral properties / dynamics at T=0:

$$A^{\mathcal{O}}(\omega) = -\frac{1}{\pi} \lim_{\eta \to 0} \left\langle \psi_0 \left| \mathcal{O}^\dagger \frac{1}{\omega - H + E_0 + i\eta} \mathcal{O} \right| \psi_0 \right\rangle = \sum_n |\langle \psi_n | \mathcal{O} | \psi_0 \rangle|^2 \delta[\omega - (E_n - E_0)]$$

complete spectrum !?

Way out: Kernel Polynomial & Maximum Entropie Methods

1 Expansion of $\delta[\ldots]$ – series of Chebyshev polynomials $T_m(x)$:

$$A^{\mathcal{O}}(x) = \frac{1}{\pi\sqrt{1-x^2}} \left(\mu_0^{\mathcal{O}} + 2 \sum_{m=1}^{M=\infty} \mu_m^{\mathcal{O}} T_m(x) \right)$$

2 Determination of moments: $\mu_m^{\mathcal{O}} = \int_{-1}^{1} dx\, T_m(x) A^{\mathcal{O}}(x) = \langle \psi_0 | \mathcal{O}^\dagger T_m(X) \mathcal{O} | \psi_0 \rangle$.

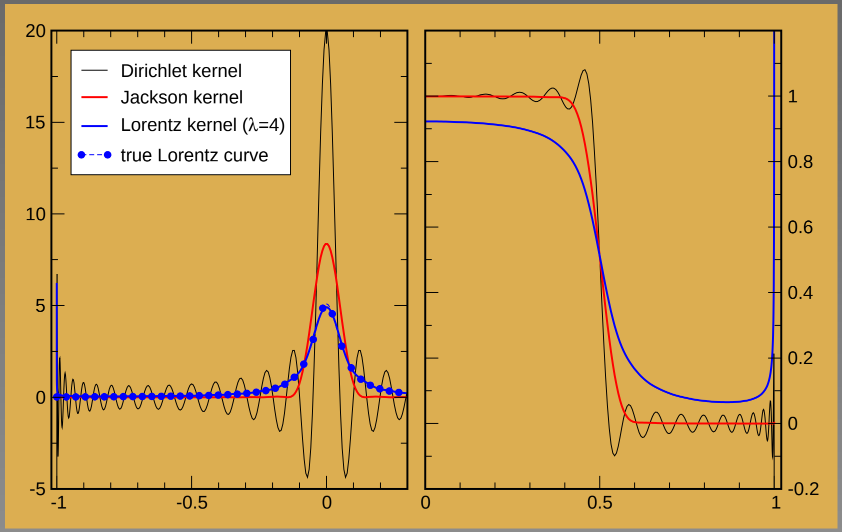
by iterative MVM, where $X = (H - b)/a$, i.e. $E_n \in [-1, 1]$ and $M < \infty$.

3 Reconstruction of $A^{\mathcal{O}}(x)$ from M moments (FFT) via linear approximation (KPM) or nonlinear optimization (MEM).

I. 3. Kernel polynomials & Gibbs oscillations

✗ Problem: M finite
$\leadsto$ truncation errors!

✓ Solution: damping factors,
e.g., Jackson or Lorentz kernels



Advantages of KPM:

uniform reconstruction of spectra – gap features	high-resolution applications	CPU-time $(\propto MD)$ "trace" – average over $\|r\rangle$

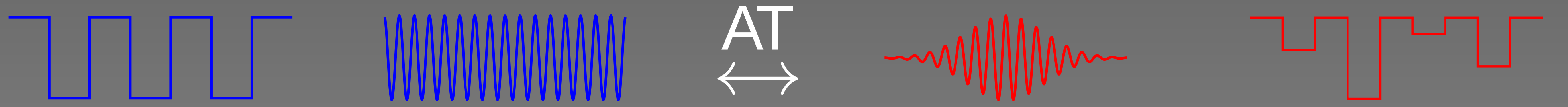
► **Recent improvements:**

- generalisation to multivariate case $\leadsto$ finite-temperature (dynamical) correlation functions
- combination with other techniques (Cluster Perturbation Theory ($N \rightarrow \infty$), ...)

Weiße, Alvermann, Schubert, Wellein, Fehske (review (RMP?) $\longrightarrow$ many applications)

II.1. Anderson transition

periodic crystal | extended states | localised states | disordered material

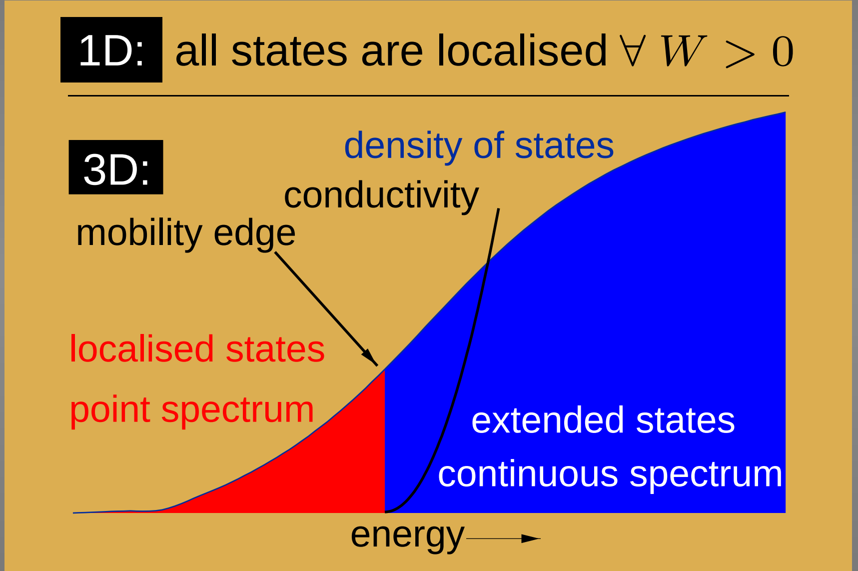


Bloch theorem | "metal" | "insulator" | impurity scattering

generic model:

$$\hat{H} = \sum_{j=1}^{N} \epsilon_j \hat{c}_j^\dagger \hat{c}_j - t \sum_{\langle jk \rangle} \left(\hat{c}_j^\dagger \hat{c}_k + \hat{c}_k^\dagger \hat{c}_j \right)$$

$$p(\epsilon_j) = \frac{1}{W}\, \theta\left(\frac{W}{2} - |\epsilon_j| \right)$$



✗ Problem: Calculating quantities which characterise the localisation transition,

$$|\psi(r)| \propto e^{-r/\lambda} \quad , \quad \sigma_{\mathrm{dc}} \propto \mathrm{Tr}[\hat{v}\, \mathrm{Im}\{\hat{G}\}\, \hat{v}\, \mathrm{Im}\{\hat{G}\}] \quad , \quad P_{ij}(t \to \infty) \propto |\hat{G}_{ij}^R|^2 \quad , \ldots$$

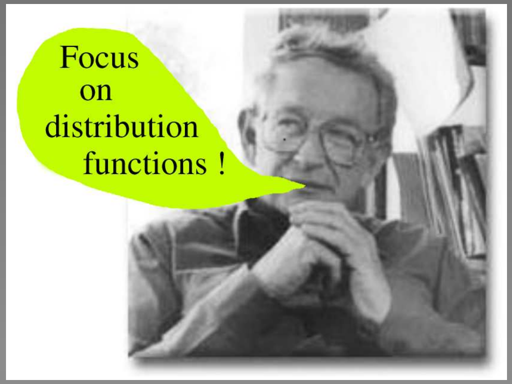
is an extremely difficult task, especially in the presence of interactions!

All simple attempts give diffusion!

II.2. Local distribution approach

Most mean values, e.g. $\langle$DOS$\rangle$, contain almost no information about AT!

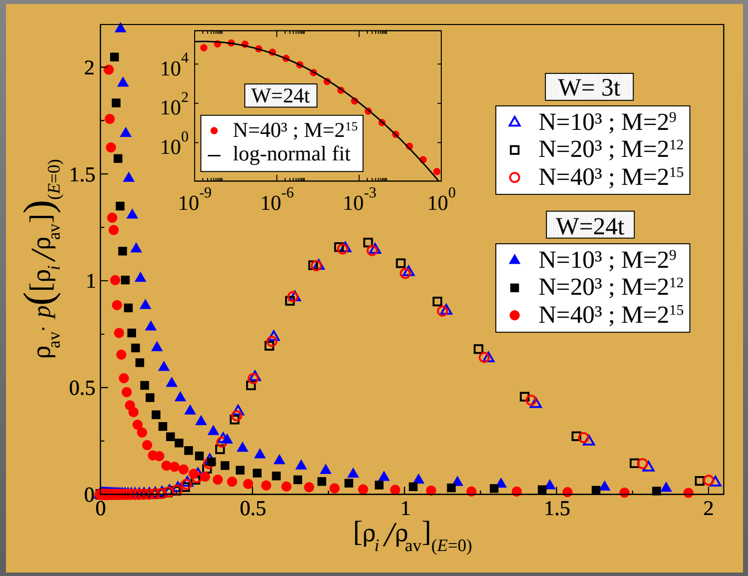
How to proceed?



▶ **LDOS:** $\rho_i = \sum_{n=1}^{N} |\psi_n(\mathbf{r}_i)|^2 \delta(E - E_n)$

- obtained efficiently by KPM
- random sample generation $\rightsquigarrow$ $p(\rho_i)$
- distribution $p(\rho_i)$ critical at AT
- $W \nearrow$: normal → log-normal → singular

LDOS distribution density for $E = 0$:



Characterisation of the distribution?

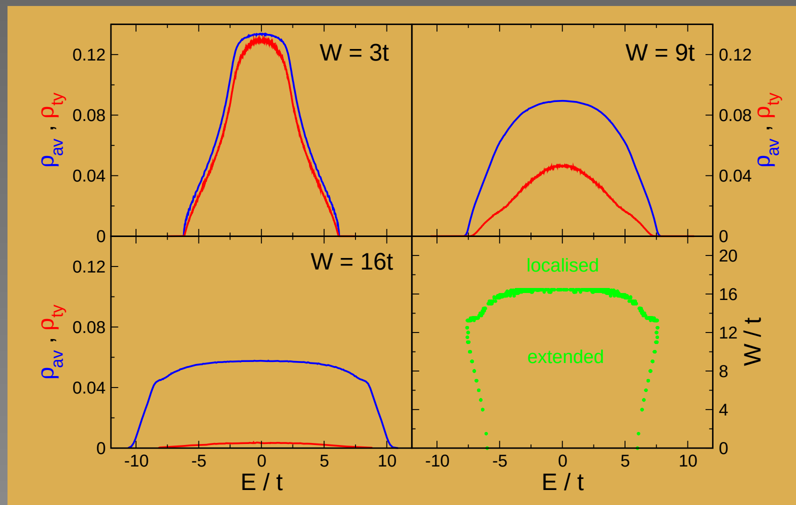
arithmetic mean $\rho_{\text{av}} = \langle \rho_i \rangle$ inappropriate

geometric mean $\rho_{\text{ty}} = \exp\langle \ln \rho_i \rangle$ suitable

$$\langle \ldots \rangle = \frac{1}{K_r K_s} \sum_{\text{samples}}^{K_r} \sum_{\text{sites}}^{K_s} \ldots$$

(typical values: $K_r \times K_s = 10^4 \times 100$)

II.3. Mean & Typical DOS



Anderson transition

$\rho_{\rm ty}(E) \to 0$ for $W \to W_c$

typical DOS $\rightsquigarrow$ "order parameter" !

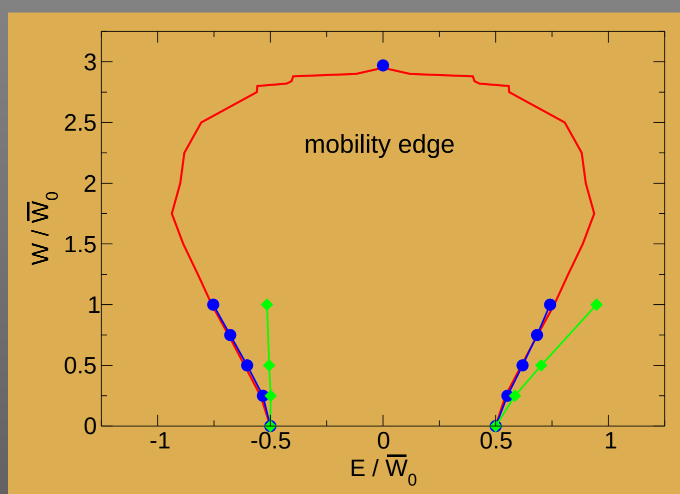
Comparison with other results:

$\rho_{\rm ty}$ – localisation criterion of

equal quality and accuracy!

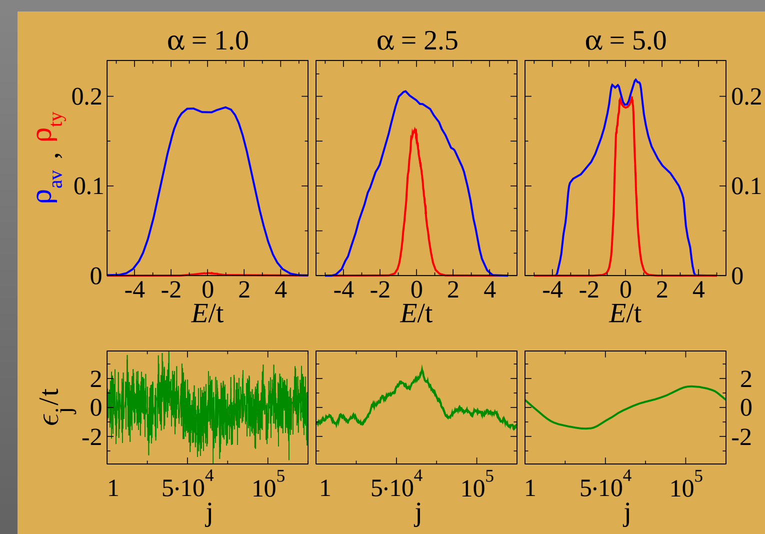
Influence of electron-phonon coupling

$H^{\rm ep} = g\omega_0 \sum (b_i^\dagger + b_i) n_i$ (BL - AAT)



Correlated disorder $\mathcal{F}(\langle \epsilon_i \epsilon_j \rangle) \propto k^{-\alpha}$

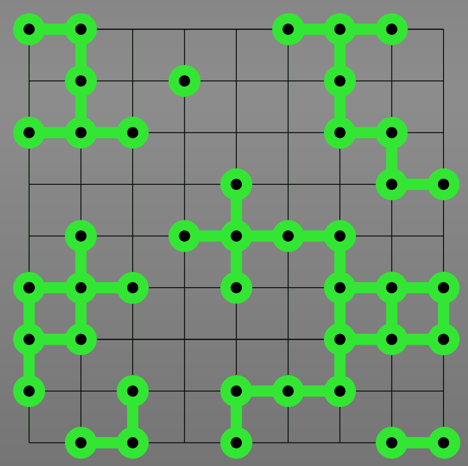
(transport in biological molecules)



II.4. Quantum percolation

classically:

- percolation $\hat{=}$ geometric problem
- $p < p_c$: only finite clusters
- $p > p_c$: $\exists$ infinite cluster A_∞



site percolation:

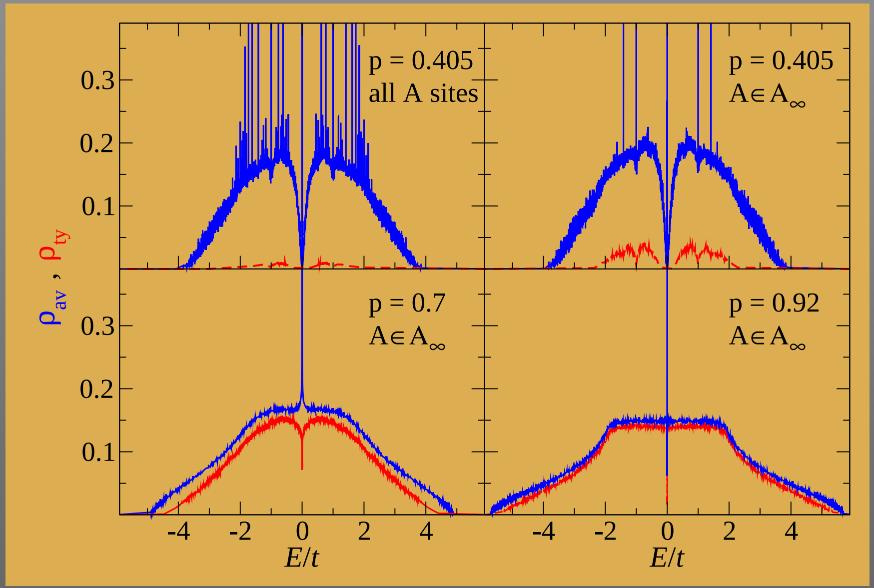
$$p(\epsilon_i) = p\,\delta(\epsilon_i - \epsilon_A) + (1-p)\,\delta(\epsilon_i - \epsilon_B)$$

limit: $\epsilon_B - \epsilon_A \to \infty$

quantum-mechanically:

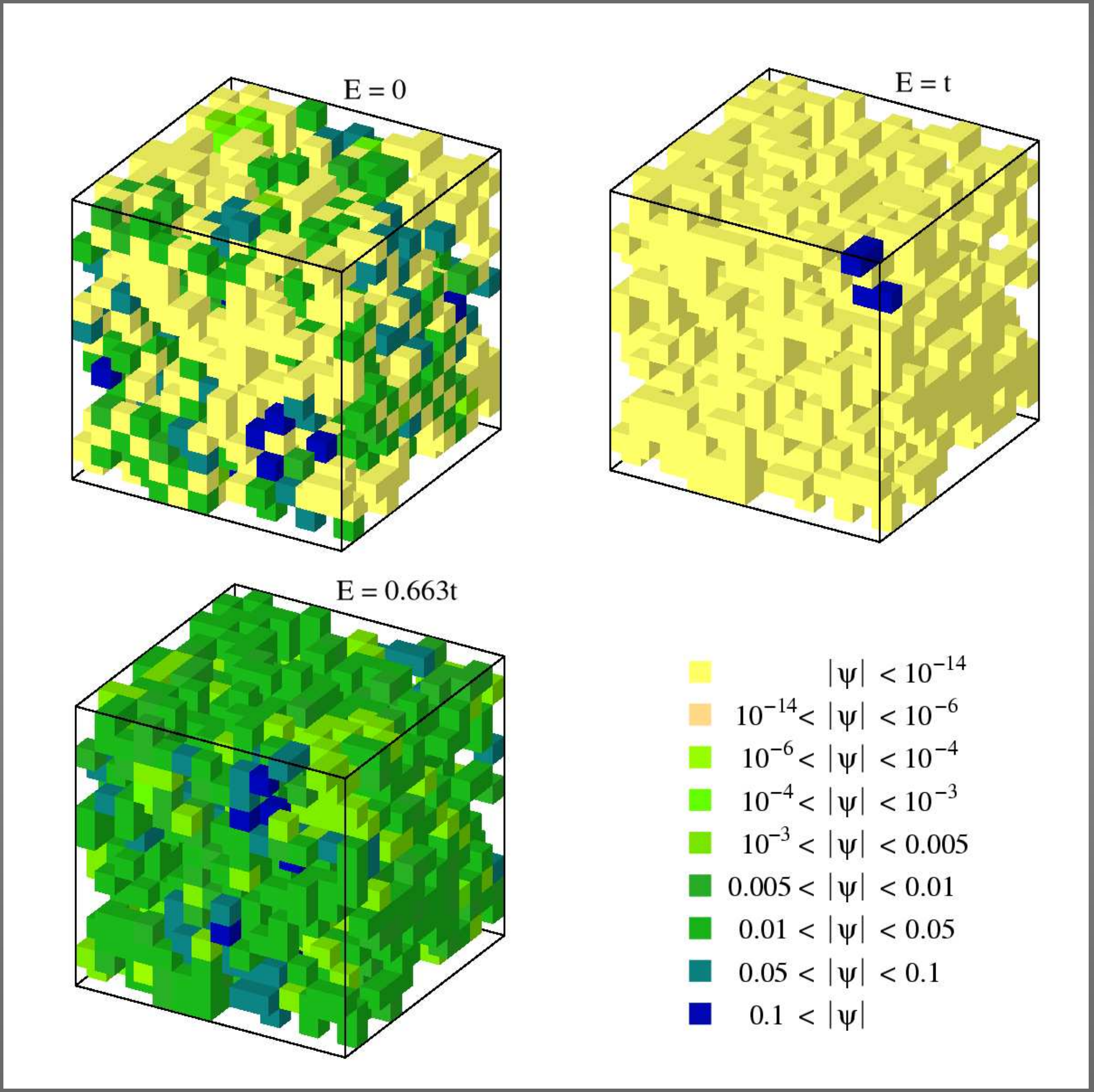
- tunneling effects $\rightsquigarrow p_q < p_c$
- localisation effects $\rightsquigarrow p_q > p_c$

$\hookrightarrow$ spanning cluster does not guarantee transport!



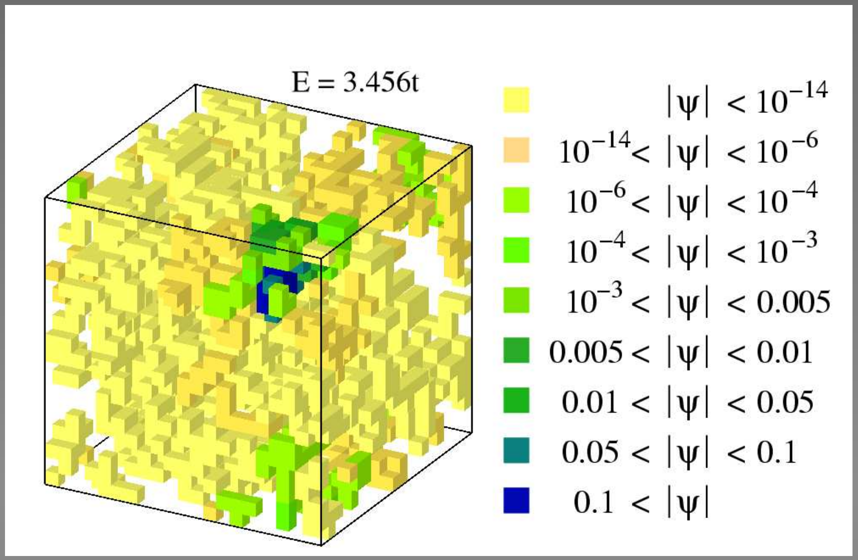
$N_\infty \approx 68000$, PBC, $M = 2^{15}$, $K_s \times K_r = 32 \times 32$

II.5. Amplitudes of wave functions

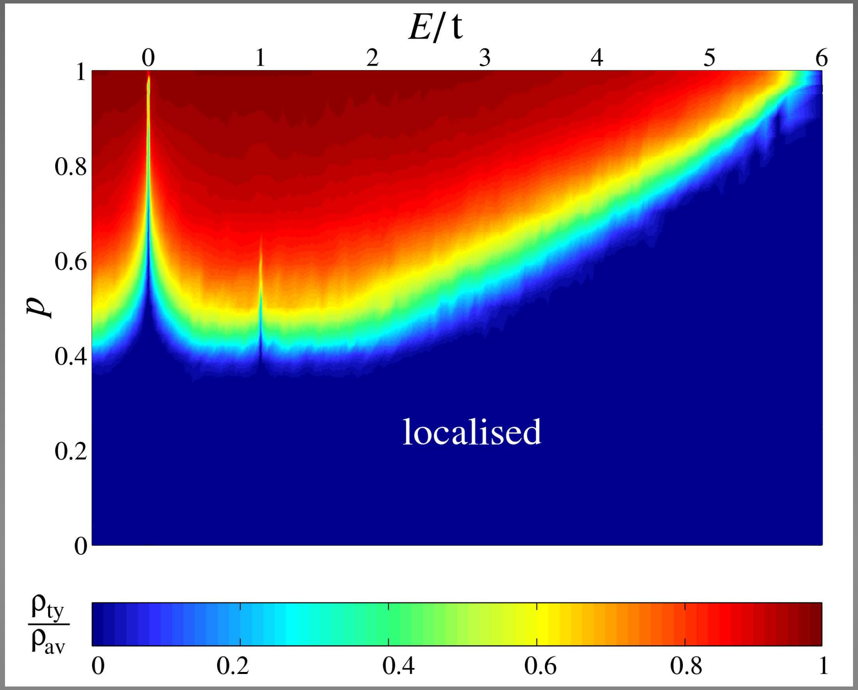


$p = 0.45 > p_c$, $N = 14^3$, PBC, restriction to A_∞, ED

II.6. Nature of states



$p = 0.33 \gtrsim p_c$, $N = 21^3$, PBC, restriction to A_∞, ED



$N = 100^3$ (50^3), for $p < 0.5$ $(p > 0.5)$, PBC, $M = 2^{14}$, $K_s \times K_r = 32 \times 32$

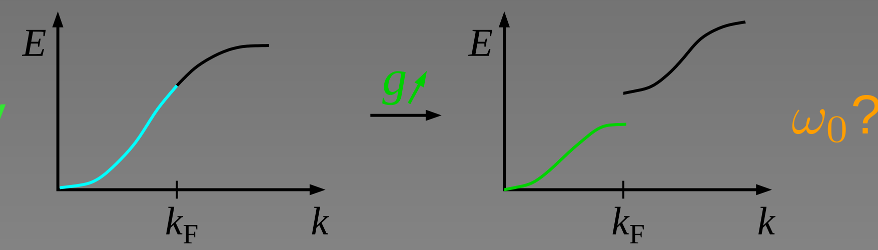
- $p_q > p_c$
- fragmentation of spectrum into extended & localised states
- anomalous localised states within band (band centre!)

Surprisingly rich physics!

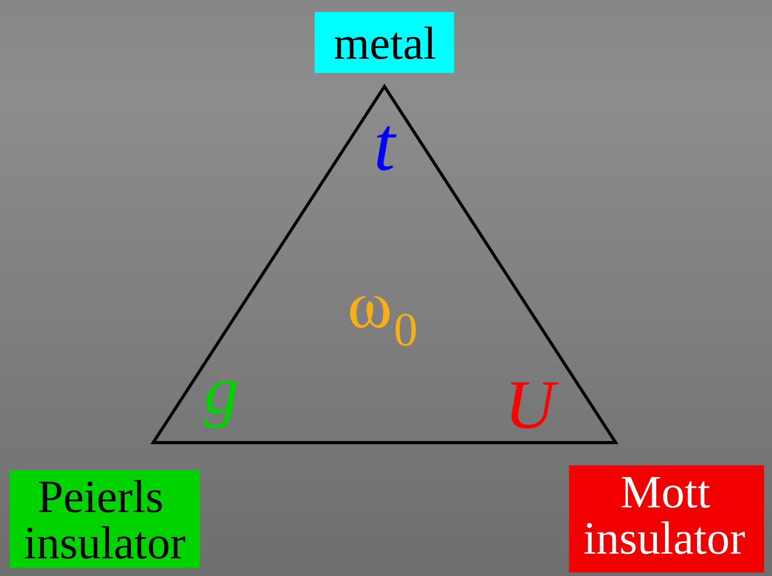
III.1. Low-D strongly correlated e-ph systems

- quasi-1D materials – very susceptible to structural distortions
  commensurate band fillings $\rightarrow$ symmetry broken ground states

  $n = 1$ - famous example : Peierls instability



general scenario:



- excitations:
  - electron-hole pairs

$\hookrightarrow$ quasiparticle behaviour

- excitations:
  - charge - massive
  - spin - gapless

$\hookrightarrow$ spin- charge separation

Quantum phase transitions at $T = 0$?

► 1D : Fermi liquid picture breaks down! $\rightsquigarrow$ **Spinless fermion Holstein model**

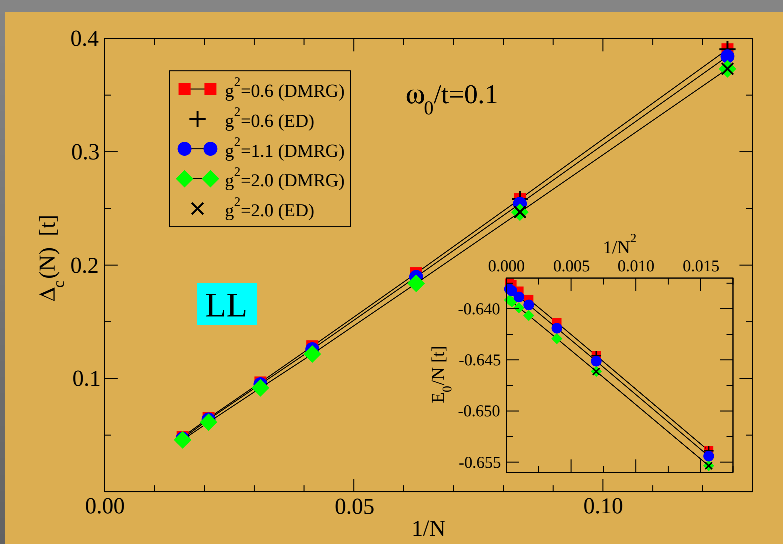
conformal field theory → scaling relations

$$\varepsilon_0(\infty) - \frac{E_0(N)}{N} = \frac{\pi}{3}\frac{u_\rho}{2}\frac{1}{N^2}$$

$$\Delta_c(N) = E_0^{(\pm 1)}(N) - E_0(N) = \pi\,\frac{u_\rho}{2}\,\frac{1}{K_\rho}\,\frac{1}{N}$$

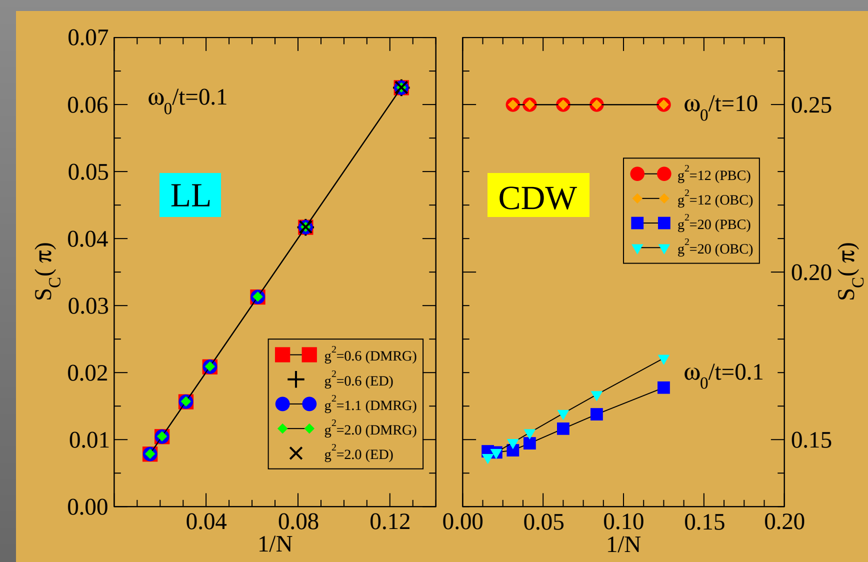
DMRG → nonuniversal **LL parameters:**

charge velocity u_ρ, interaction exponent K_ρ



charge structure factor:

$$S_c(\pi) = \frac{1}{N^2}\sum_{i,j}(-1)^j\langle(n_i - \tfrac{1}{2})(n_{i+j} - \tfrac{1}{2})\rangle$$

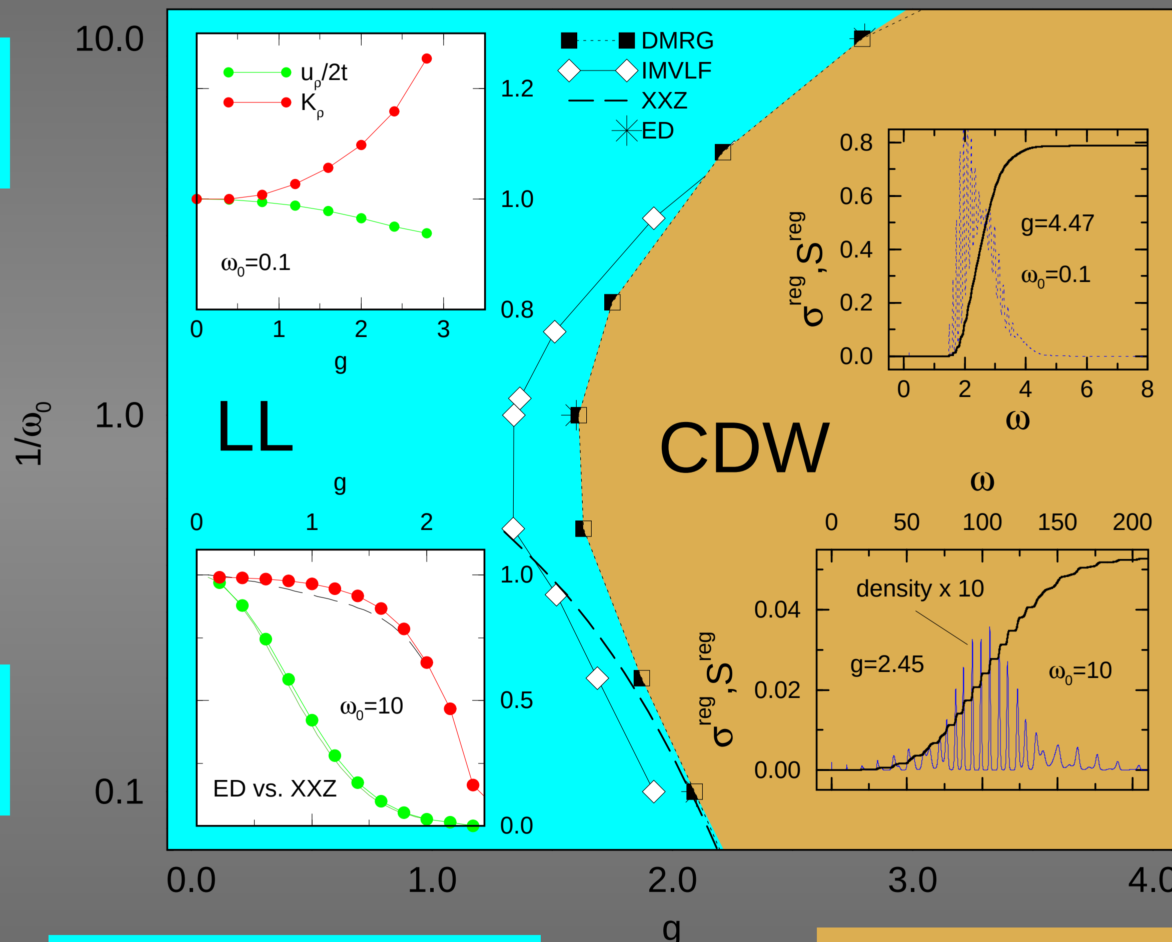


no LRO **LRO**

- Lattice dynamical effects → charge density wave formation above $g_c(\omega_0)$!

attractive LL

repulsive LL



Peierls distorted state

metallic behaviour

activated transport

$u_\rho,\ K_\rho$

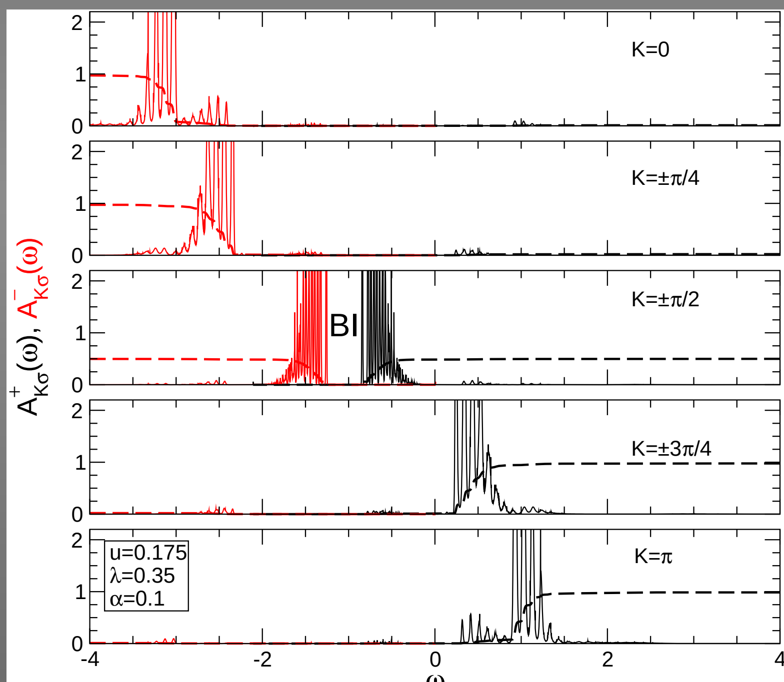
$$\sigma^{reg}(\omega) = \frac{\pi}{N} \sum_{m \neq 0} \frac{|\langle \psi_0 | \hat{j} | \psi_m \rangle|^2}{E_m - E_0}\, \delta(\omega - E_m + E_0)$$

III.4. Band insulator vs. Polaronic superlattice

- strong EP coupling regime + spin → **Holstein Hubbard model** (half filling)
- (inverse) photoemission spectra:

$$A^{\pm}_{K\sigma}(\omega) = \sum_m |\langle\psi_m^{(N_{el}\pm1)}|c^{\pm}_{K\sigma}|\psi_0^{(N_{el})}\rangle|^2 \delta[\omega \mp (E_m^{(N_{el}\pm1)} - E_0^{(N_{el})})]$$

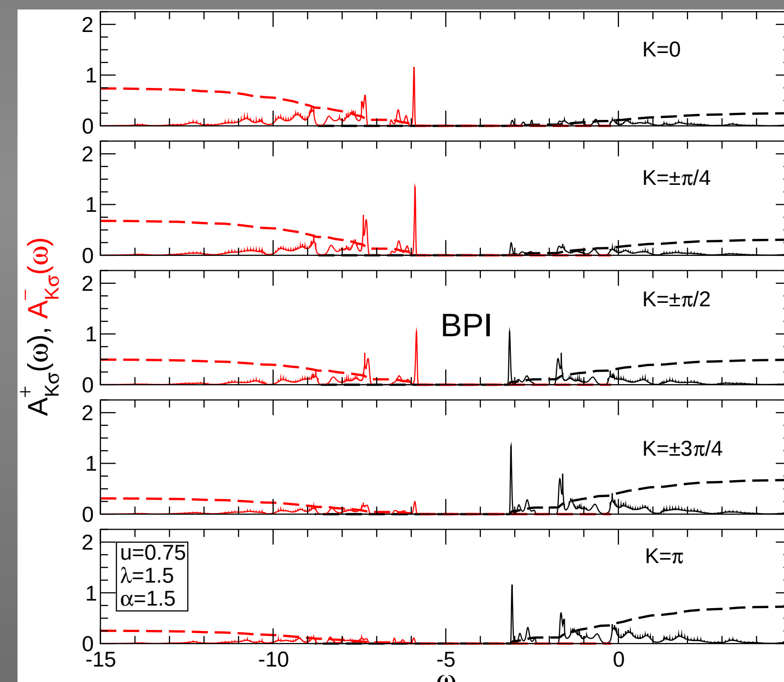
adiabatic case: $\omega_0/t \ll 1$

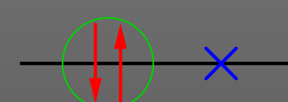


“traditional” Peierls band insulator

dispersion $\propto \epsilon_k$ + gap feature

antiadiabatic case: $\omega_0/t \gg 1$

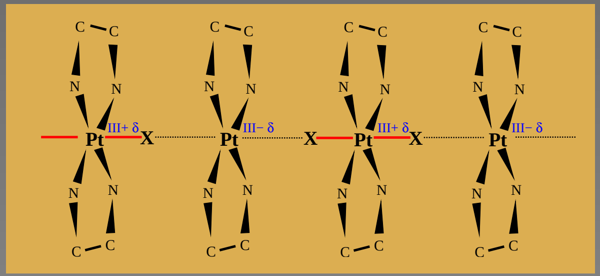


self-trapping  + ordering

dispersionsless band, low spectral weight

III.5. Intrinsic localised vibrational modes

MX-chains: strong CDW



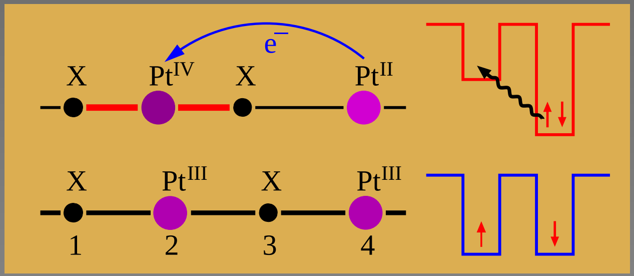
Peierls-Hubbard model

EP-coupling

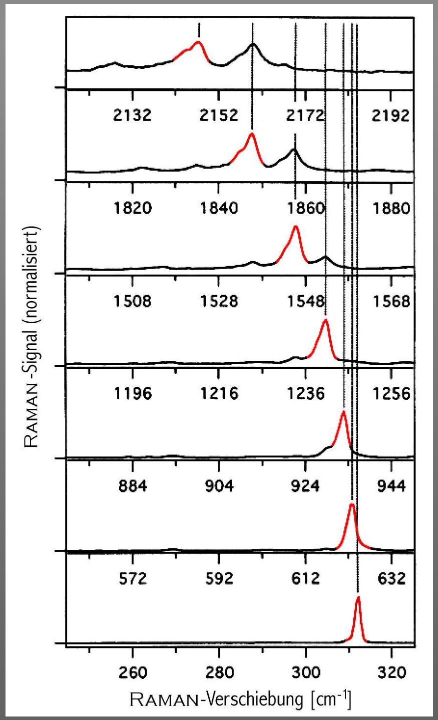
$$\propto \lambda_R (b_R + b_R^\dagger)(n_{e,2} - n_{e,4})$$

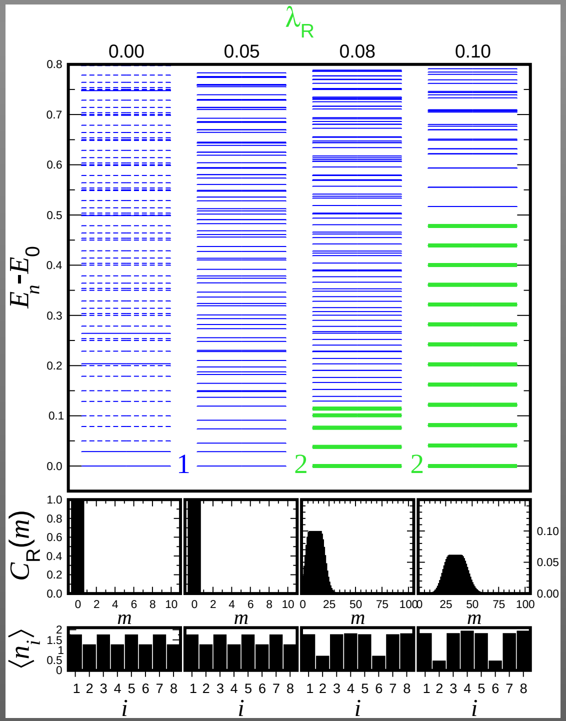
non-linear dynamics

$[\mathrm{Pt(en)_2}][\mathrm{Pt(en)_2Cl_2}](\mathrm{ClO_4})_4$



Resonance Raman spectra (Swanson et. al., PRL '99) $\longrightarrow$ redshift of overtones!





$$r_n = \frac{n\omega_R^{(1)} - \omega_R^{(n)}}{\omega_r^{(1)}}$$

n	$r_n^{\text{exp.}}$	$r_n^{\text{theo.}}$
2	0.4	0.4
3	1.1	1.1
4	2.4	2.5
5	4.6	4.7
6	7.7	7.5
7	11.6	11.2

✓

III.6. Peierls insulator vs. Mott insulator

▶ **Inclusion of Coulomb repulsion ?**

- many-body excitation gaps:

$$\Delta_c = E_0^{(N_{el}+1)}(\tfrac{1}{2}) + E_0^{(N_{el}-1)}(-\tfrac{1}{2}) - 2E_0^{(N_{el})}(0)$$

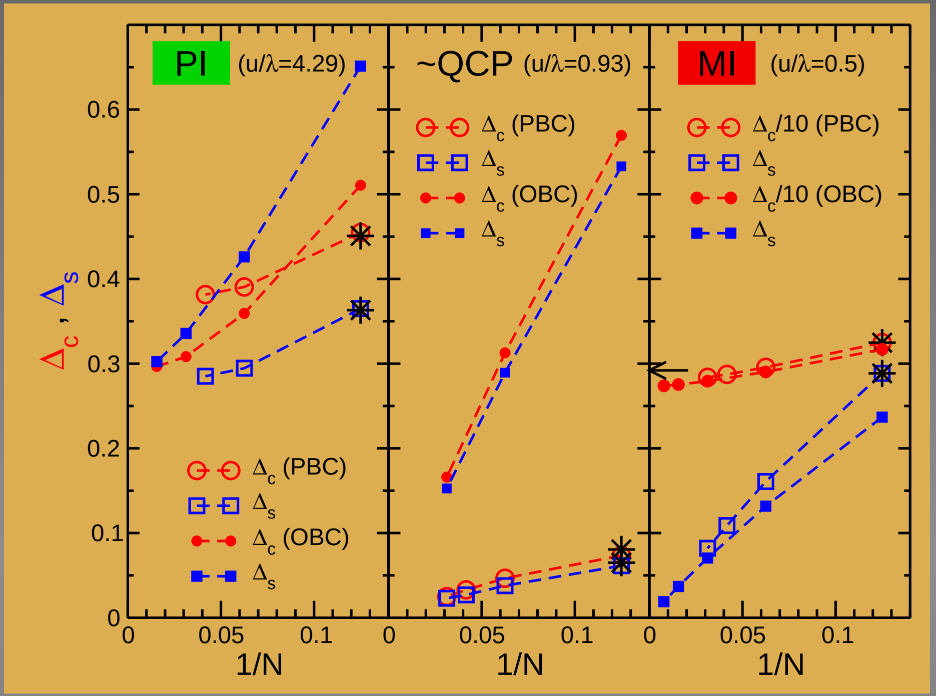
$$\Delta_s = E_0^{(N_{el})}(1) - E_0^{(N_{el})}(0)$$

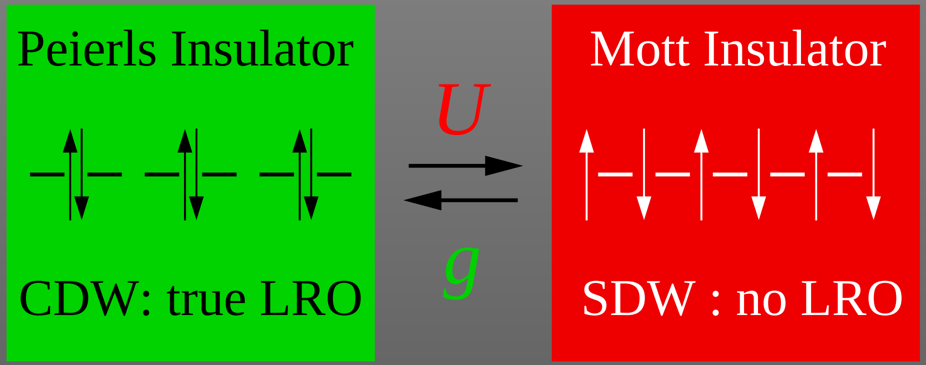
- charge - & spin structure factors

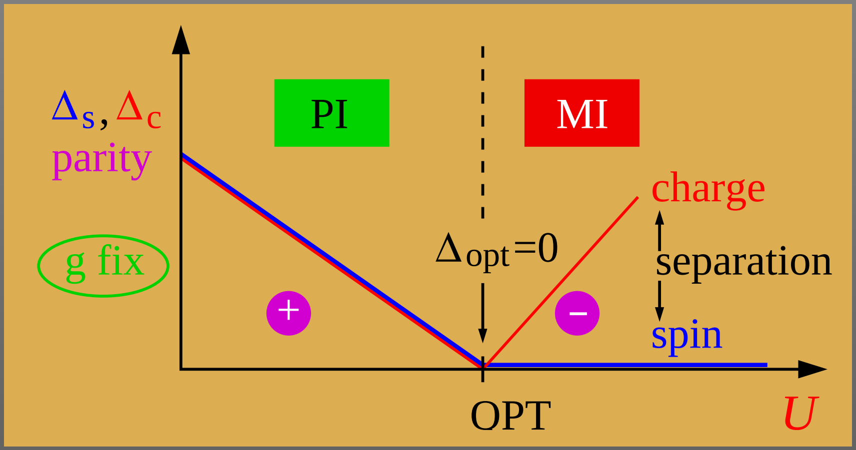
DMRG + finite-size scaling

$\longrightarrow$ detection of

quantum phase transition!



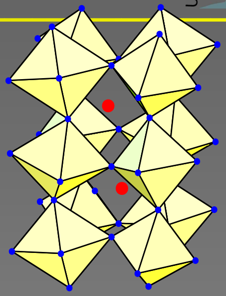


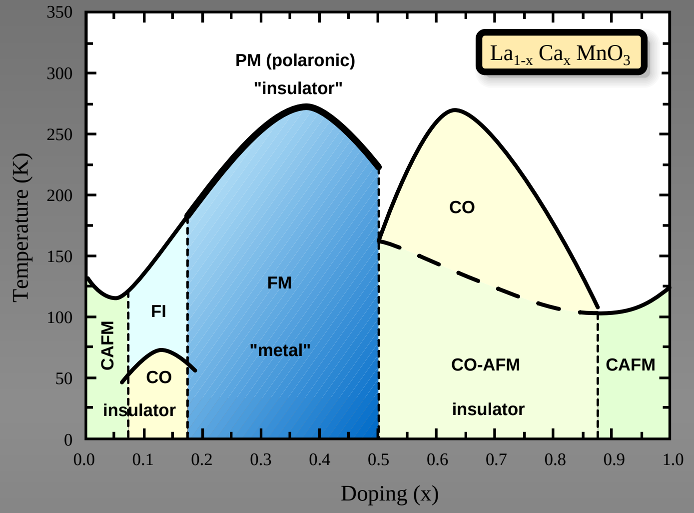


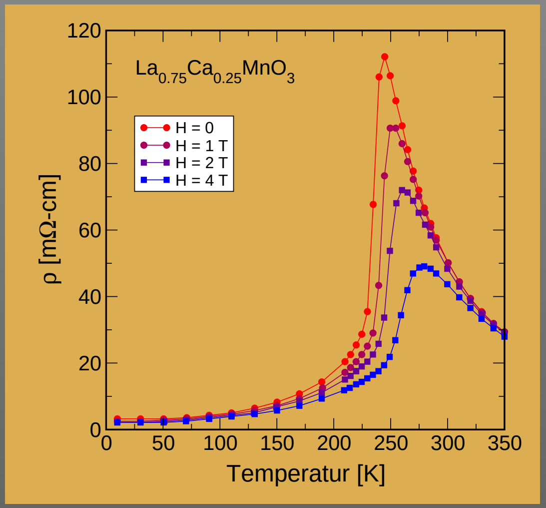
IV.1. What is interesting about manganites?

► Mixed-valence manganese oxides $R_{1-x}A_xMnO_3$

(R = La, Pr, Nd ; A = Ca, Sr, Ba) $[R^{3+}Mn^{3+}, A^{2+}Mn^{4+}]$





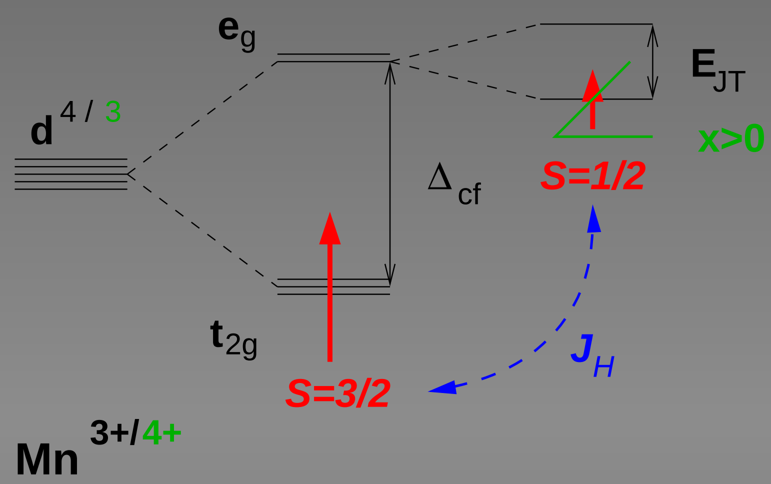


- rich electronic, magnetic & structural phase diagram
- colossal negative magnetoresistance near T_c
- enormous technological potential (sensors, spin electronic, devices)

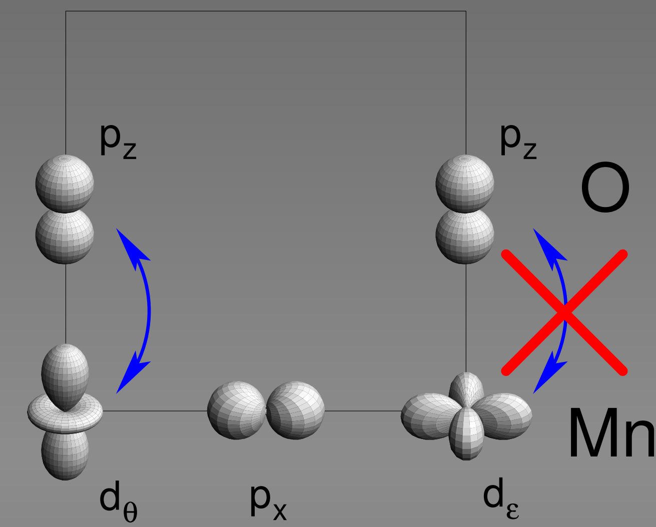
- Challenge for solid state theory:
- strong electron-phonon correlations
- relevance of orbital degrees of freedom

IV.2. Microscopic modelling

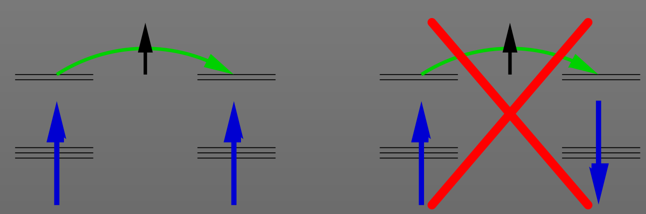
- electronic structure ($U \gg 1$)



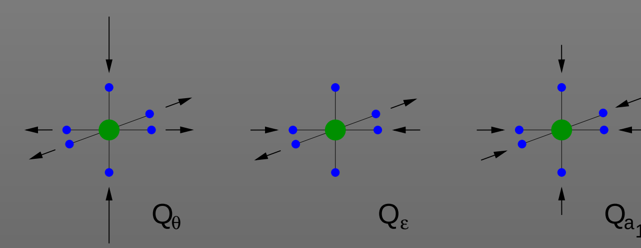
- orbitals (anisotropic hopping)



- ferromagnetic double exchange ($J_h > 1$)



- phonons (JT & breathing)



Weiße, Fehske, New. J. Phys. (Focus Review), ***6****, 158 (2004)*

IV.3. Effective low energy Hamiltonian

$$H = \sum_{i,\delta} R_\delta \left(H^{1,z}_{i,i+\delta} + H^{2,z}_{i,i+\delta} \right) + H^{\rm ep}$$

$$H^{1,z}_{i,j} = -\frac{t}{4}\left(a_{i,\uparrow}a^\dagger_{j,\uparrow} + a_{i,\downarrow}a^\dagger_{j,\downarrow}\right) d^\dagger_{i,\theta} n_{i,\varepsilon} d_{j,\theta} n_{j,\varepsilon} + \text{H.c.} \quad \propto \text{double exchange}$$

$$\begin{aligned}
H^{2,z}_{i,j} &= t^2 \, \frac{\vec{S}_i \vec{S}_j - 4}{8} \left[\frac{(4U + J_h)\, P^\varepsilon_i P^\theta_j}{5U(U + \frac{2}{3}J_h)} + \frac{(U + 2J_h)\, P^\varepsilon_i P^\varepsilon_j}{(U + \frac{10}{3}J_h)(U + \frac{2}{3}J_h)} \right] - t^2 \, \frac{\vec{S}_i \vec{S}_j + 6}{10(U - 5J_h)} \, P^\varepsilon_i P^\theta_j \\
&+ t_\pi^2 \, \frac{\vec{S}_i \vec{S}_j - 3}{3} \left[\frac{(U - 2J_h)(R_x(P^\varepsilon_i P^{a_2}_j) + R_y(P^\varepsilon_i P^{a_2}_j))}{\frac{19}{3}J_h(2U - \frac{7}{3}J_h)} + \frac{(U + \frac{5}{3}J_h)(R_x(P^\theta_i P^{a_2}_j) + R_y(P^\theta_i P^{a_2}_j))}{\frac{13}{3}J_h(2U - J_h)} \right] \\
&+ t_\pi^2 \, \frac{\vec{S}_i \vec{S}_j - 4}{8} \left[\frac{R_x(P^\varepsilon_i P^\varepsilon_j) + R_y(P^\varepsilon_i P^\varepsilon_j)}{U + 8J_h/3} + \frac{R_x(P^\theta_i P^\theta_j) + R_y(P^\theta_i P^\theta_j)}{U + 2J_h} \right. \\
&+ \left. \frac{(2U + \frac{14}{3}J_h)(R_x(P^\varepsilon_i P^\theta_j) + R_y(P^\varepsilon_i P^\theta_j))}{(U + 4J_h)(U + \frac{2}{3}J_h)} \right] + t^2 \, \frac{\vec{S}_i \vec{S}_j - 3}{32 J_h} \, P^\varepsilon_i P^{a_2}_j + t_\pi^2 \, \frac{\frac{4}{9}\vec{S}_i \vec{S}_j - 1}{U + \frac{4}{3}J_h} \, P^{a_2}_i P^{a_2}_j + \text{H.c.}
\end{aligned}$$

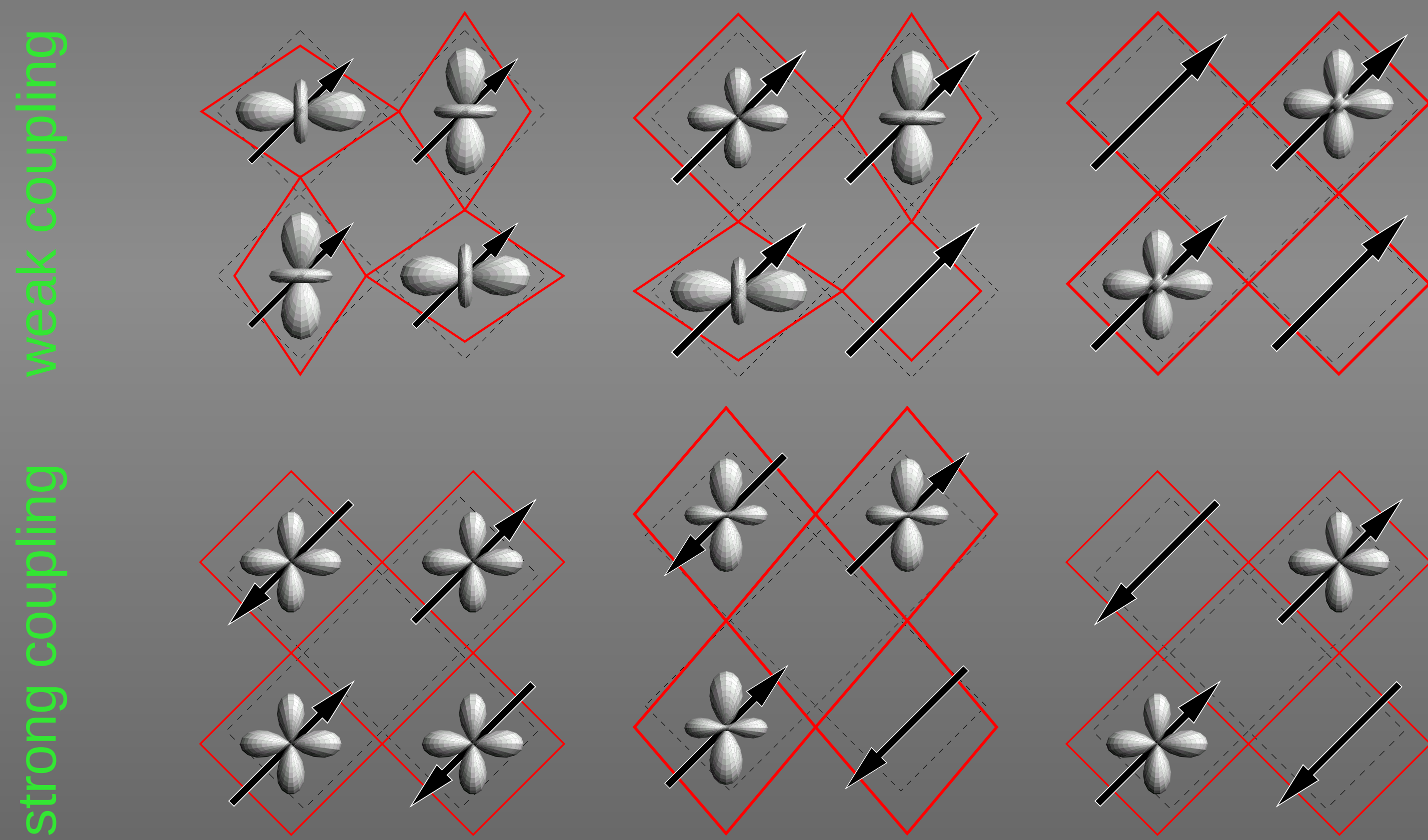
$$\begin{aligned}
H^{\rm ep} &= g \sum_i \left[(n_{i,\varepsilon} - n_{i,\theta})(b^\dagger_{i,\theta} + b_{i,\theta}) + (d^\dagger_{i,\theta} d_{i,\varepsilon} + d^\dagger_{i,\varepsilon} d_{i,\theta})(b^\dagger_{i,\varepsilon} + b_{i,\varepsilon}) \right] \\
&+ \tilde{g} \sum_i (n_{i,\theta} + n_{i,\varepsilon} - 2n_{i,\theta} n_{i,\varepsilon})(b^\dagger_{i,a_1} + b_{i,a_1}) + \omega \sum_i \left[b^\dagger_{i,\theta} b_{i,\theta} + b^\dagger_{i,\varepsilon} b_{i,\varepsilon} \right] + \tilde{\omega} \sum_i b^\dagger_{i,a_1} b_{i,a_1}
\end{aligned}$$

IV.4. Short-range correlations

exact cluster calculations $\rightarrow$ correlation functions $\rightarrow$ SRO patterns

($U = 6$eV, $J_H = 0.7$eV, $t = 3t_\pi = 0.4$eV, $\omega_0 = \tilde{\omega}_0 = 0.07$eV, $g/\omega_0 = 0.5$ ... 3)

doping: $x = 0$ $x = 0.25$ $x = 0.5$



EP interaction $\rightarrow$ orbital order $\rightarrow$ spin order $\rightarrow$ transport

IV.5. Percolative mixed-phase description

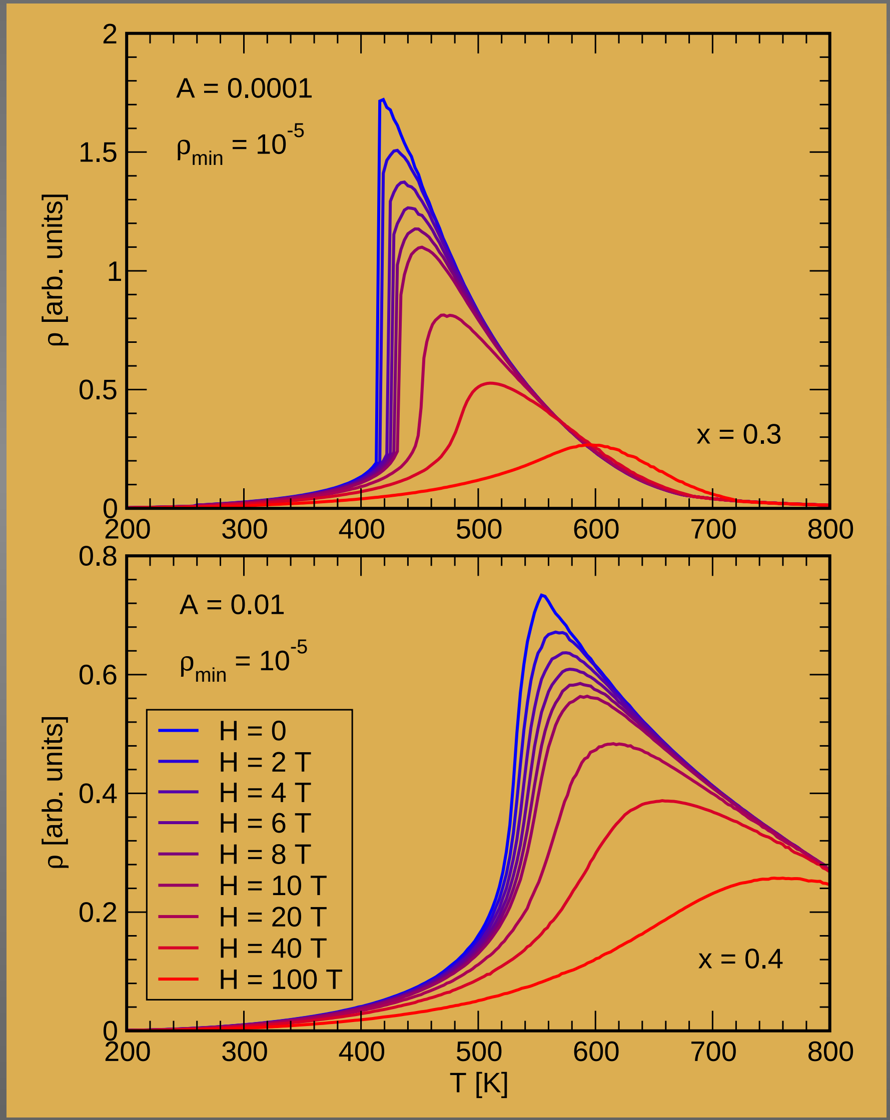
- Exp.: spatial coexistence of conducting and insulating regions both above and below T_c
- Theory: phase separation approaches, ... ?

↪ Proposal: Two-phase scenario with percolative characteristics!

$$\pi^{(f)} = \pi^{(p)} = \pi_{\text{eq}}$$

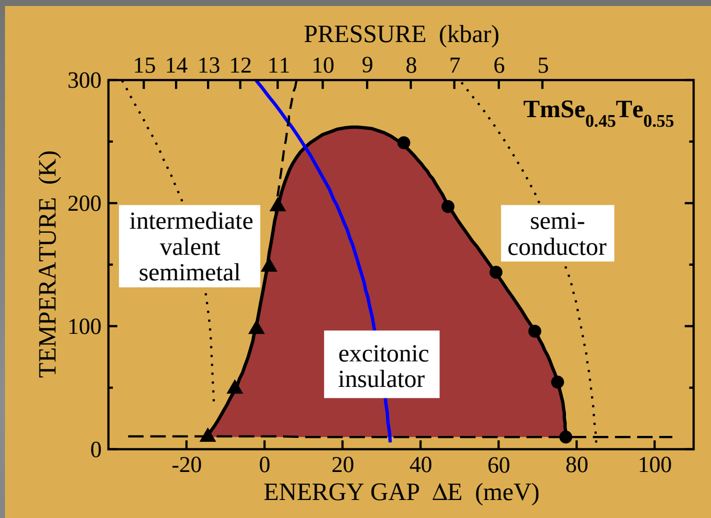
- FM metallic component
  $\rho^{(f)} = \frac{B}{x^{(f)}}(\rho_S + \rho_{\text{min}})$
- polaronic insulating component
  $\rho^{(p)} = \frac{A}{\beta x^{(p)}}\rho_S \exp(-\beta\epsilon_p)$

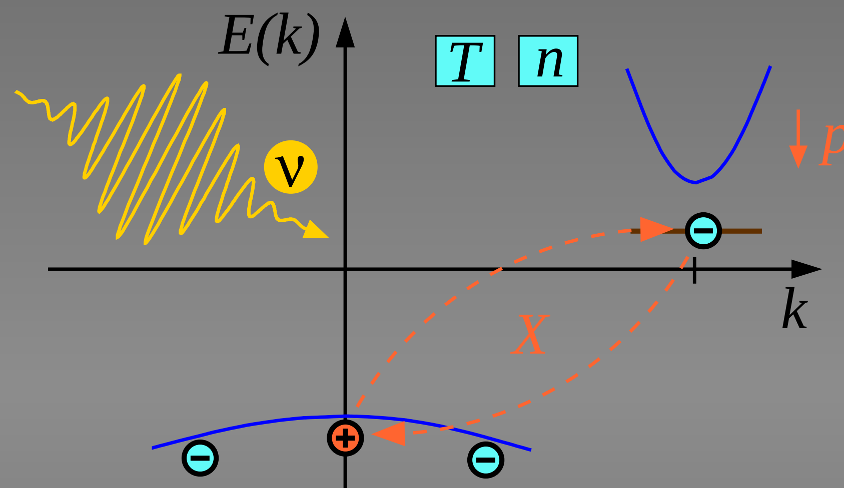
$$\rho_S = \rho_S[S, z, B_S(z), \coth[S, z]\,]$$

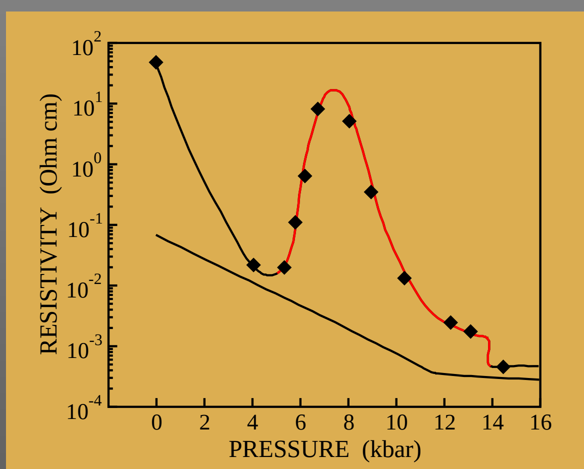


V.1. Two-component Coulomb systems

Motivation: pressure-driven semiconductor → excitonic insulator → semimetal transition in Tm[Te,Se] alloy systems (ETH group, PRL ’91, PRB ’04)







real substance: “unconventional” semiconductor

- mixed valence ($4f^{13}5d^0 \rightleftharpoons 4f^{12}5d^1$)
- coupling to phonons
- strong local Coulomb correlations (f-band)

$\hookrightarrow m_h \gg m_e$

$\rightsquigarrow$ investigation of mass-asymmetric e$^-$–hole plasmas

V.2. Characterisation of complex plasmas

length scales:	energy scales:	coupling parameters:	degeneracy:
$\bar{r} \sim n^{-d}$, Λ $a_B \propto \frac{\epsilon}{q_a q_b m_r}$	$\langle K \rangle_{\text{cl}} \propto k_B T$, $\langle K \rangle_{\text{qm}} \propto E_F$ $\langle U_c \rangle \propto \frac{q_a q_b}{\epsilon \bar{r}}$, $\langle U_c \rangle_B \propto E_B$	$\Gamma = \frac{\langle U_c \rangle}{\langle K \rangle}$ $r_s = \frac{\bar{r}}{a_B}$	$\chi = n \Lambda^d$ $\chi \sim \left(\frac{\Lambda}{\bar{r}}\right)^d$

classical systems $\xleftarrow{\chi<1}$ χ $\xrightarrow{\chi>1}$ quantum systems

ideal gas $\xleftarrow{\chi \ll 1 \ \& \ \Gamma \ll 1}$ ✓ $\xrightarrow{\chi \gg 1 \ \& \ r_s \ll 1}$ ideal quantum gas

“non-trivial” physics for $\Gamma \gtrsim 1\,;\ r_s \sim 1\,;\ \chi_i \sim 1\,;\ m_a \neq m_b$

$\hookrightarrow$ unbiased numerical techniques:

Molecular Dynamics:
Newton equations of motion

Path Integral Monte Carlo:

$$\exp\left\{-\frac{H}{k_B T}\right\} = \left[\exp\left\{-\frac{H}{M k_B T}\right\}\right]^M$$

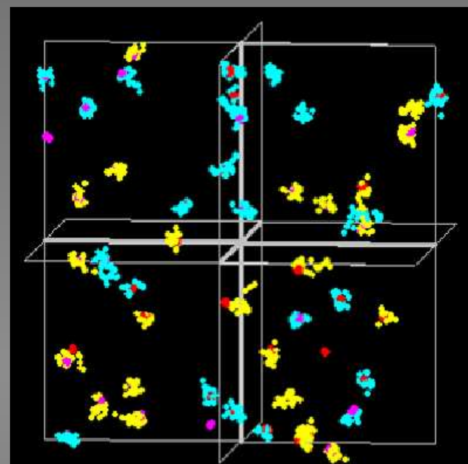
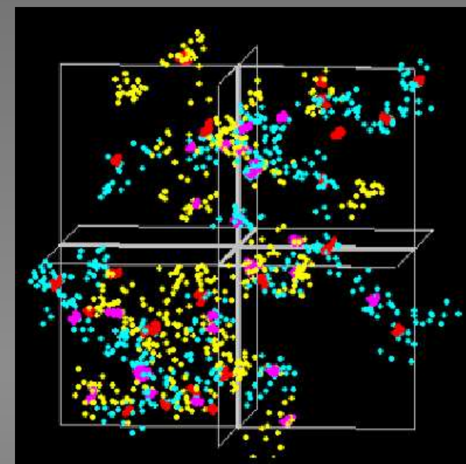
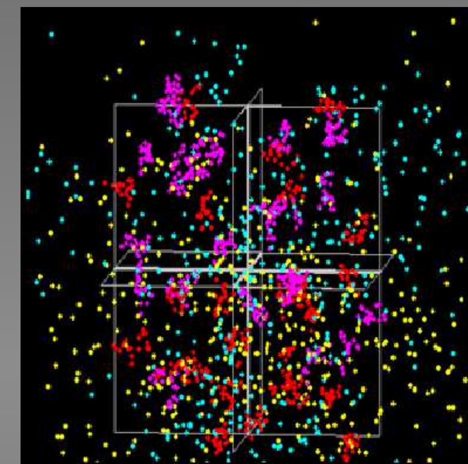
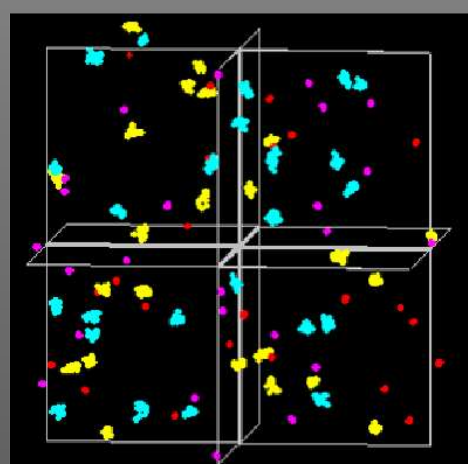
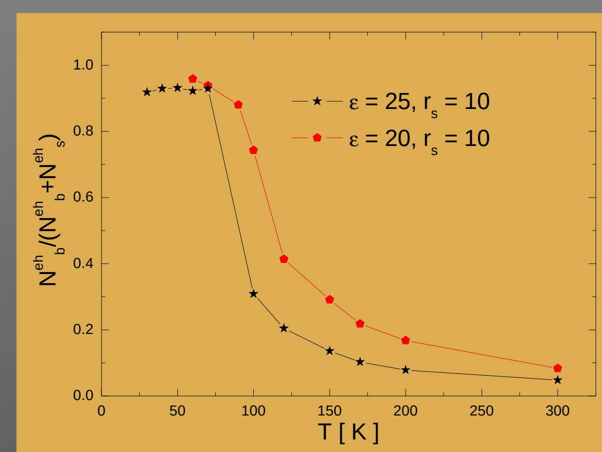
($M \gg 1 \rightsquigarrow \Gamma[\ldots] \ll 1$, Feynman)

$\hookrightarrow$ bound states $\longleftrightarrow$ collective phases $\longleftrightarrow$ electron-hole plasmas

bound states	collective phases	electron-hole plasmas
excitons	excitonic insulator	Mott transition
Bi-X, Cluster	Wigner crystal? BEC?	

V.3. Bound-state formation & Mott transition

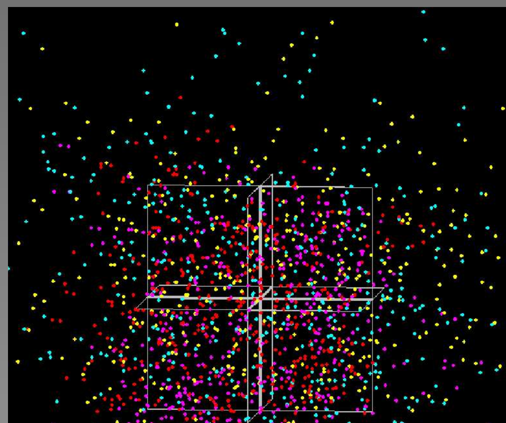
“first principle” PIMC results: (N_e=N_h=50, m_e=2, m_h=80, ϵ=20, E_B^X=50meV; Kelbg potential)

	$r_s = 10$	$r_s = 4$	$r_s = 1$
$T = 50\mathrm{K}$			
formation of:	excitons (X)	biexcitons	hole-liquid
$T = 200\mathrm{K}$			T-induced dissociation of excitons $T_c \sim 150\mathrm{K}!$

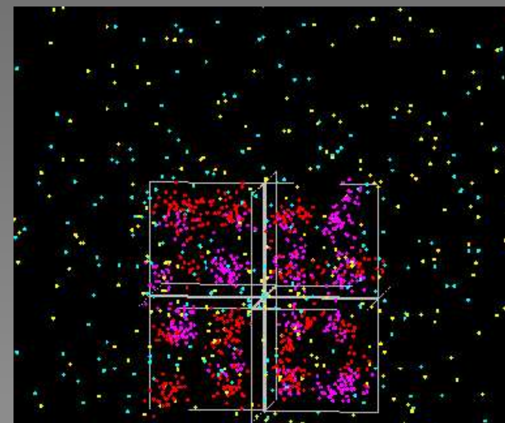
V.4. “Wigner” (Coulomb) crystallisation

Snapshots of a dense electron-hole system with $r_s = 0.63$ at $T = 0.096 E_B^X$ ($\epsilon = 1$):

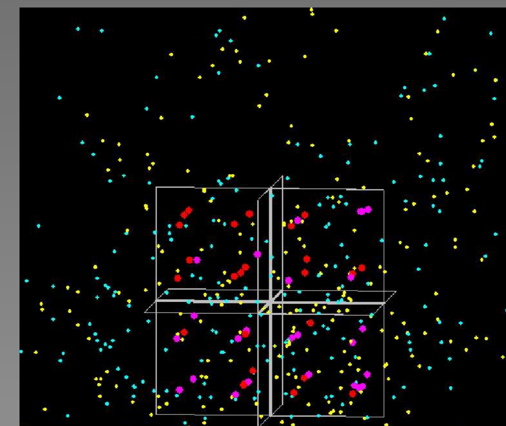
$m_h/m_e = 5$ | $m_h/m_e = 50$ | $m_h/m_e = 800$



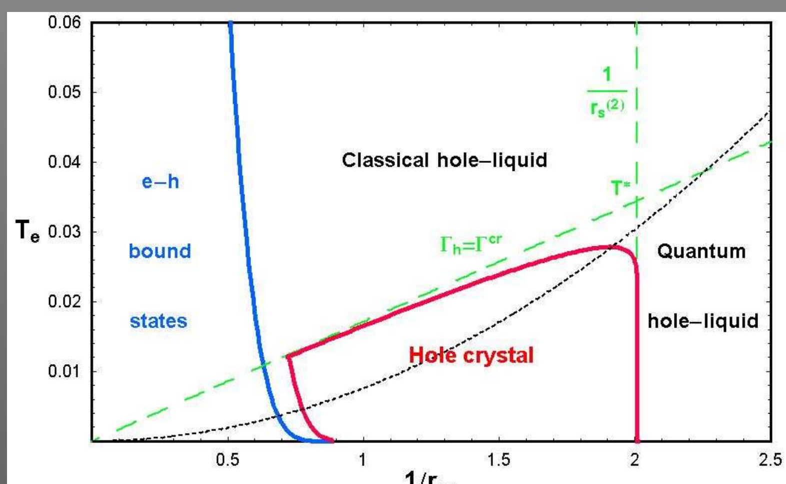
electron-hole



hole liquid



hole-crystal



$\longrightarrow$ Quantum “Wigner” crystals of holes are predicted to form in semiconductors with sufficiently flat valence bands

$(m_h/m_e)^{\mathrm{cr}} \sim 80\ (3D) \sim 30\ (2D)$

Summary

Complex interplay of order & transport phenomena

(metal $\leftrightarrow$ insulator $\leftrightarrow$ insulator transitions)

disordered systems	Anderson localisation	fragmentation of spectrum
quasi 1D materials	LL $\leftrightarrow$ Peierls $\leftrightarrow$ Mott QPT	spin-charge separation
CMR manganites	FM-metal $\leftrightarrow$ polaronic insulator	phase coexistence
e^--hole plasmas	X-formation & dissociation	“Wigner” crystallisation

Numerical study of microscopic models – powerful tool!

Quantum Monte Carlo method
Canonical ensemble

- Binary mixture of *Ne* electrons and *Ni holes*

- Partition function:

$$Z(N_e,N_i,V,\beta)=Q(N_e,N_i,\beta)/N_e!N_i!$$

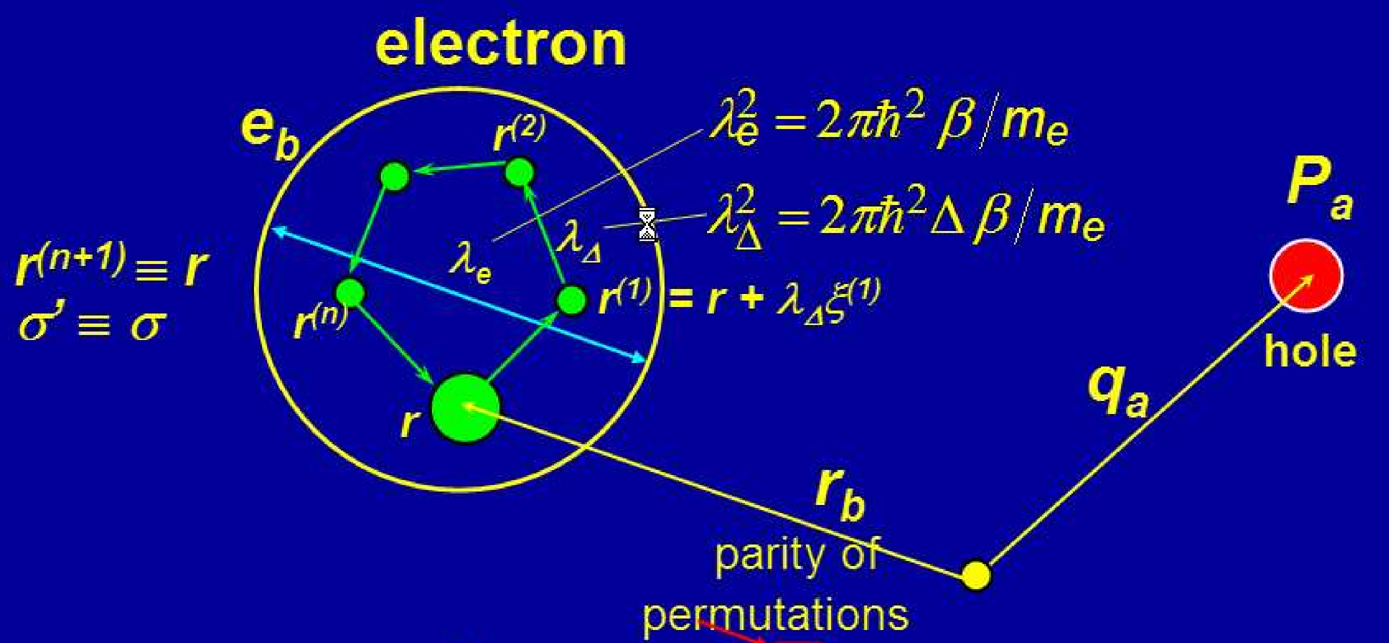
$$Q(N_e,N_i,\beta)=\sum_{\sigma}\int_V dq\,dr\,\rho(q,r,\sigma;\beta)\Big/N_e!N_i!$$

- N-particle density matrix:

$$\rho=\exp(-\beta H)=\underbrace{\exp(-\Delta\beta H)\times\ldots\times\exp(-\Delta\beta H)}_{n+1}$$

$$\beta=1/kT \qquad \Delta\beta=\beta/(n+1)$$

Path Integral representation



$$\rho(q,r,\sigma;\beta)=\frac{1}{\lambda_i^{3N_i}\,\lambda_\Delta^{3N_e}}\sum_P(-1)^{\kappa_P}\int_V dr^{(1)}\dots dr^{(n)}\times$$

$$\rho(q,r,r^{(1)};\Delta\beta)\dots\rho(q,r^{(n)},Pr^{(n+1)};\Delta\beta)S(\sigma,P\sigma'),$$

Thermal wave lengths

N-particle exchange operator

Spin matrix

«Sign problem»

$$\sum_{\sigma} \rho(q,r,\sigma;\beta) = \frac{1}{\lambda_i^{3N_i}\,\lambda_\Delta^{3N_e}} \sum_{s=0}^{N_e} \rho_s(q,[r],\beta)$$

$$\rho_s(q,[r],\beta) = \frac{C_{N_e}^{s}}{2^{N_e}} \exp\{-\beta U(q,[r],\beta)\} \prod_{l=1}^{n} \prod_{p=1}^{N_e} \phi_{pp}^{l} \det\left|\psi_{ab}^{n,1}\right|_s$$

Coulomb potential

Kelbg potential

$$U(q,[r],\beta) = U^{i}(q) + \sum_{l=0}^{n} \frac{U_l^{e}([r],\beta) + U_l^{ei}(q,[r],\beta)}{n+1}$$

Exchange matrix

$$\left\|\psi_{ab}^{n,1}\right\|_s \equiv \left\|\exp\left\{-\frac{\pi}{\lambda_\Delta^2}\left|(r_a - r_b) + y_a^{n}\right|^2\right\}\right\|_s$$

Kelbg potential

$$x_{ab} = |\mathbf{r}_{ab}| / \lambda_{ab} \qquad \lambda_{ab} = 2\pi\hbar^2 \beta / \mu_{ab}$$

$$\Phi^{ab}(x_{ab}, \Delta\beta) = \frac{e_a e_b}{\lambda_{ab} x_{ab}} \left\{ 1 - e^{-x_{ab}^2} + \sqrt{\pi}\, x_{ab} \left[1 - erf(x_{ab}) \right] \right\}$$

$|\mathbf{r}_{ab}| \to 0$:

$$\frac{\sqrt{\pi}\, e_a e_b}{\lambda_{ab}}$$

$|\mathbf{r}_{ab}| >> \lambda_{ab}$:

$$\frac{e_a e_b}{|r_{ab}|}$$

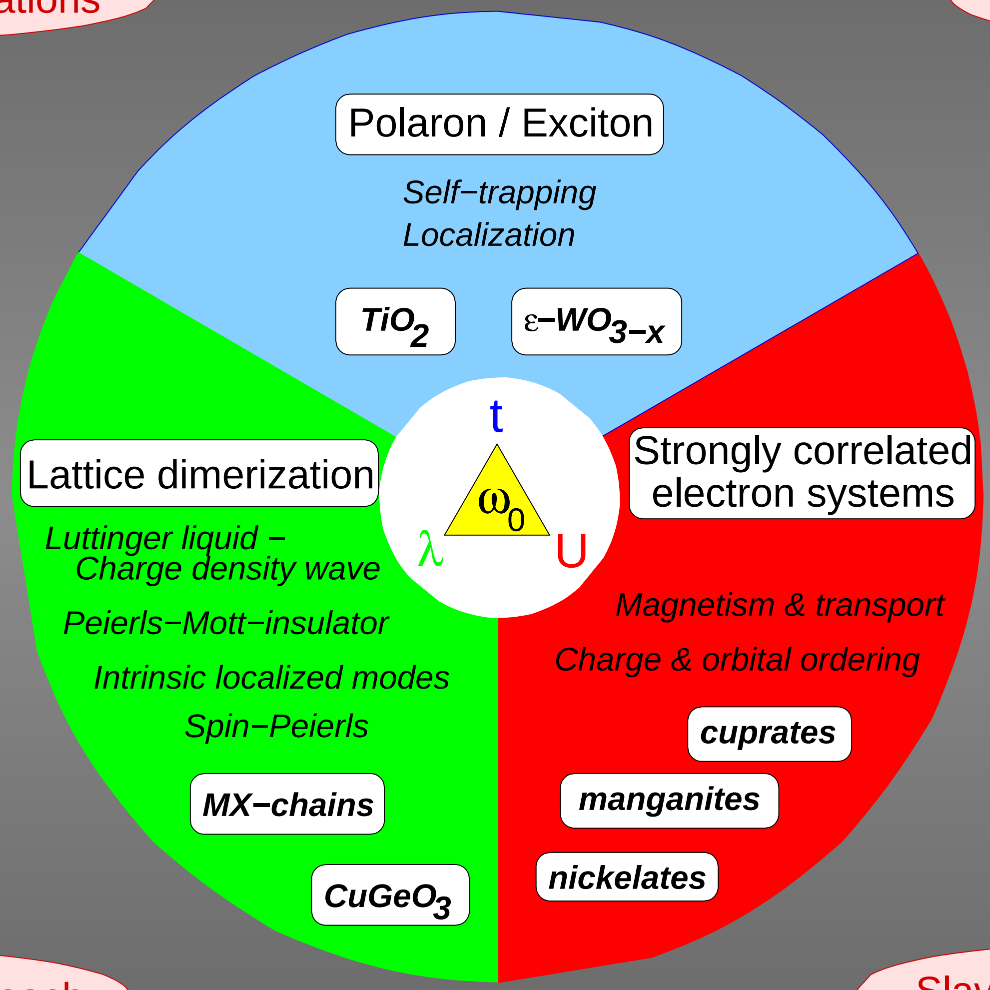
Forschungsgebiete

Unitary transformations

Statistical DMFA

Lanczos & Jacobi−Davidson diagonalization

B. Steffen
NIC Jülich



Density matrix renormalization

E. Jeckelmann
Uni Mainz

Kernel−polynomial expansion

A. Weiße
UNSW Sydney

Maximum entropy method

R. Silver
Nat. Lab. Los Alamos

Bosonization approach

Slave−field techniques