Correlated quantum particles in crystal and optical lattices

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Collaboration

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many others

Aim of this talk

CORRELATIONS

- What is it?
- How to quantify it?
- How to see it?
- Where to look for it?

Correlation

- Correlation [lat.]: con+relatio ("with relation")
- Mathematics, Statistics, Natural Science:

$$\langle xy \rangle \neq \langle x \rangle \langle y \rangle$$

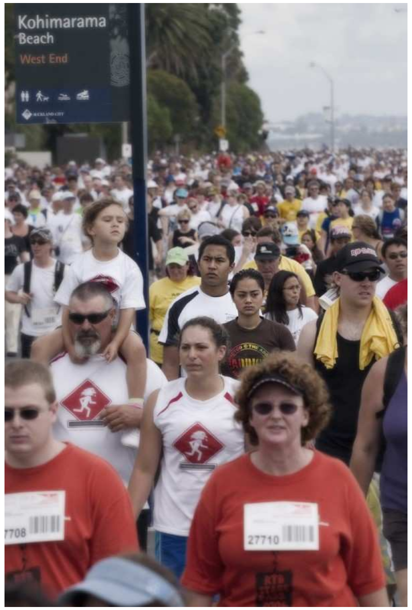
The term correlation stems from mathematical statistics and means that two distribution functions, $f(x)$ and $g(y)$, are not independent of each other.

- In many body physics: correlations are effects beyond factorizing approximations

$$\langle \rho(r,t)\rho(r',t') \rangle \approx \langle \rho(r,t) \rangle \langle \rho(r',t') \rangle,$$

as in Weiss or Hartree-Fock mean-field theories

Spatial and temporal correlations everywhere



car traffic

air traffic

human traffic

electron traffic

more .....

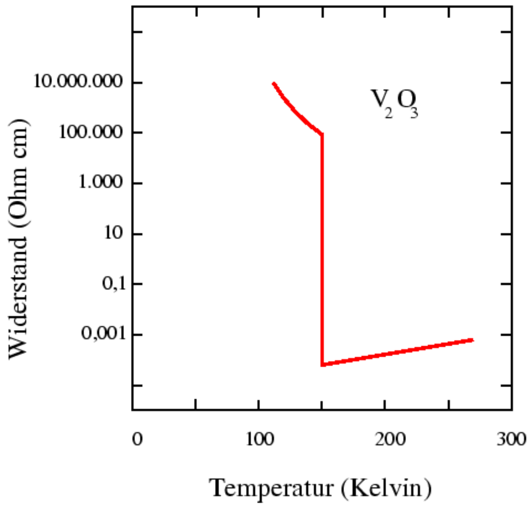


Abb. 3: Beispiel eines Metall-Isolator-Übergangs: Bei Abkühlung unter eine Temperatur von ca. 150 Kelvin erhöht sich der elektrische Widerstand von metallischem Vanadiumoxid (V_2O_3) schlagartig um das Einhundertmillionenfache (Faktor 10^8) – das System wird zum Isolator.

Spatial and temporal correlations neglected

time/space average insufficient

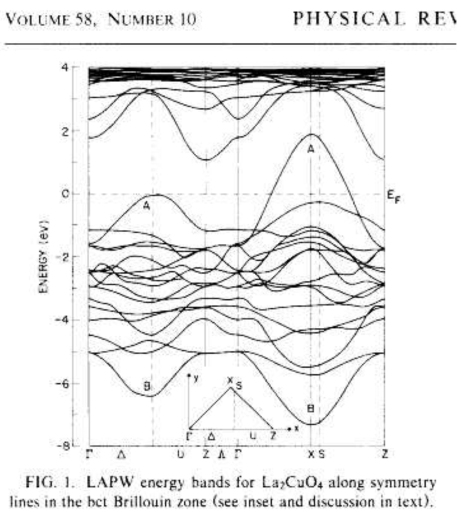
$$\langle \rho(r,t)\rho(r',t') \rangle \approx \langle \rho(r,t) \rangle \langle \rho(r',t') \rangle = \text{disaster!}$$

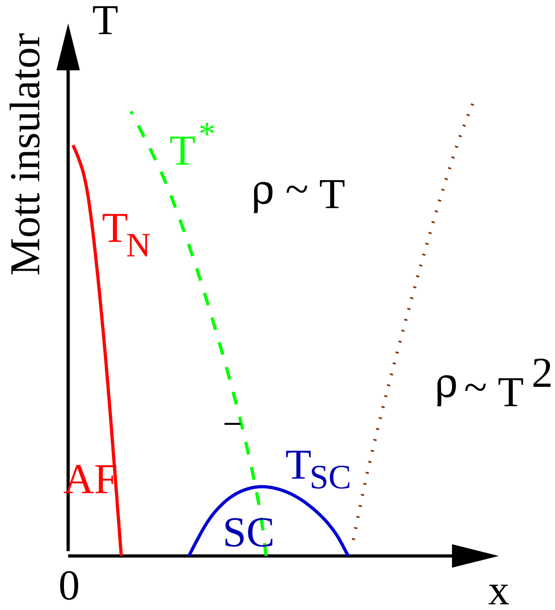
Boeing 757 and Tupolev 154 collided at 35,400ft. in 2001

Pilot of Tupolev received at the same time two conflicting (uncorrelated) instructions

Spatial and temporal correlations neglected

Local density approximation (LDA) disaster in HTC

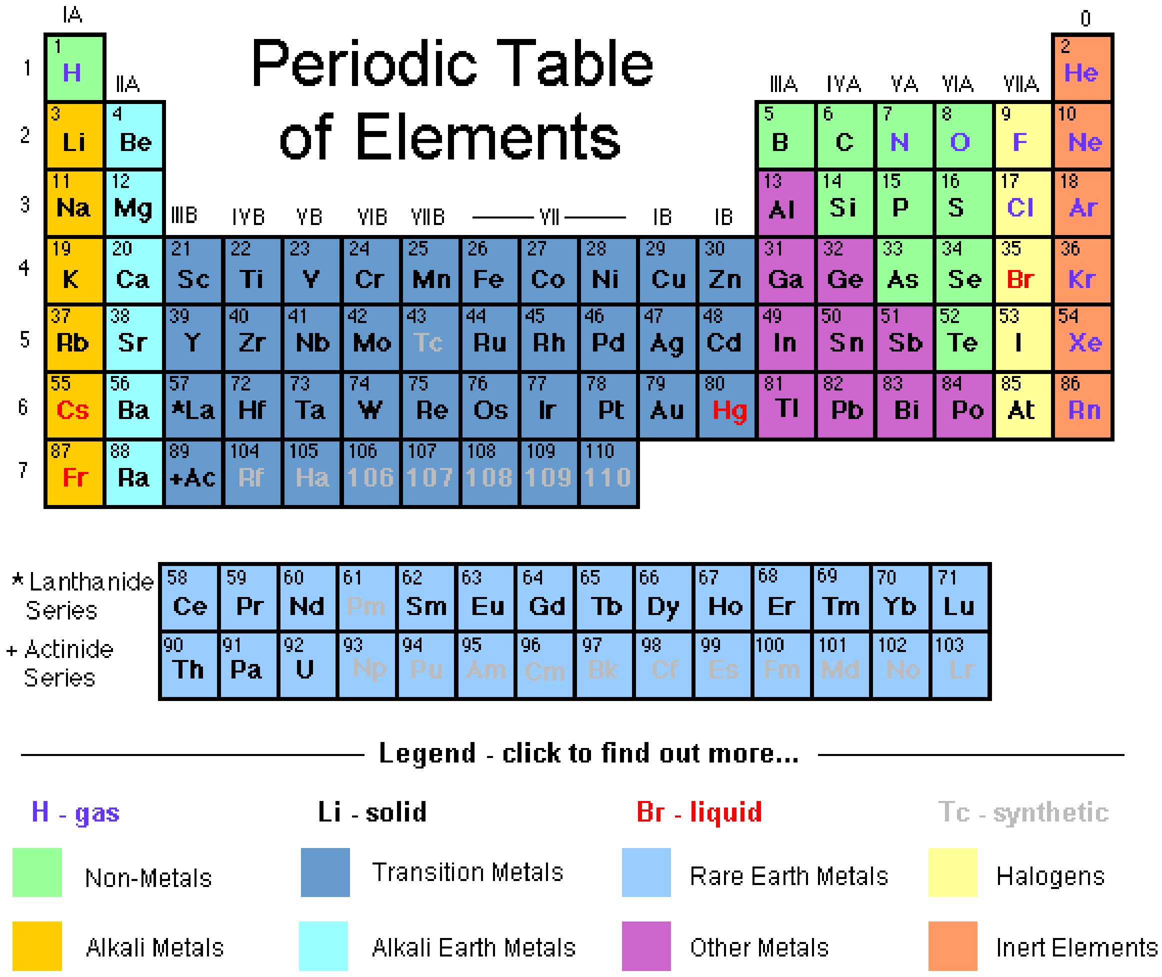




$LaCuO_4$ Mott (correlated) insulator predicted to be a metal

Partially curred by (AF) long-range order ... but correlations are still missed

Correlated electrons

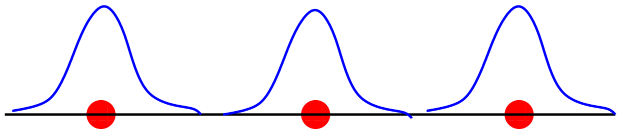


Narrow d,f-orbitals/bands $\rightarrow$ strong electronic correlations

Electronic bands in solids

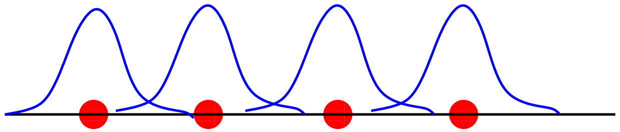
Wave function overlap $\sim t_{ij} = \langle i|\hat{T}|j\rangle \rightarrow |E_{\mathbf{k}}| \sim \mathrm{bandwidth}\ W$

Band insulators, e.g. NaCl



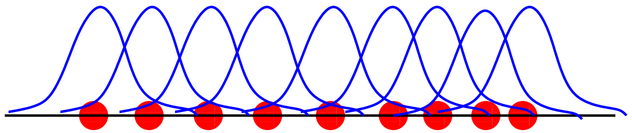
Atomic levels, localized electrons $|\mathbf{R}_i\sigma\rangle$

Correlated metals, e.g. Ni, V_2O_3, Ce



Narrow bands, $|\mathbf{R}_i\sigma\rangle \leftrightarrow |\mathbf{k}\sigma\rangle$

Simple metals, e.g. Na, Al



Broad bands, extended Bloch waves $|\mathbf{k}\sigma\rangle$

Electronic bands in solids

Mean time τ spent by the electron on an atom in a solid
depends on the band width W

$$\text{group velocity} \quad v_{\mathbf{k}} \approx \frac{\text{lattice spacing}}{\text{mean time}} = \frac{a}{\tau}$$

$$\text{Heisenberg principle} \quad W\tau \sim \hbar$$

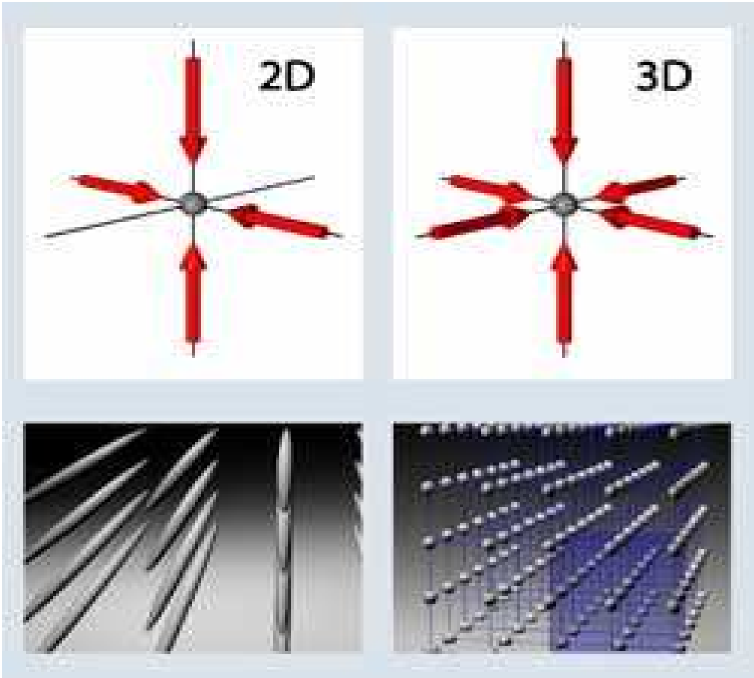
$$\frac{a}{\tau} \sim \frac{aW}{\hbar} \Longrightarrow \tau \sim \frac{\hbar}{W}$$

Small W longer interaction with another electron on the same atom
Strong electronic correlations

Optical lattices filled with bosons or fermions

Greiner et al. 02, and other works

atomic trap and standing waves of light create optical lattices $a \sim 400 - 500nm$

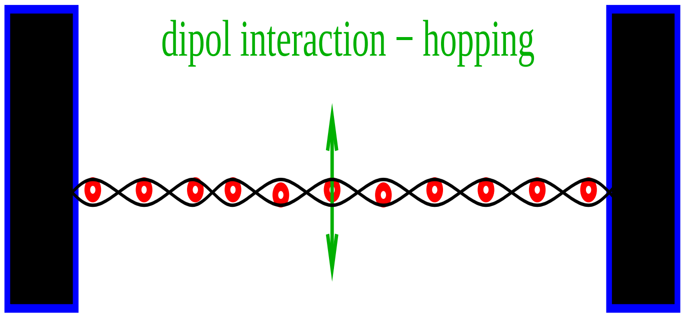


alkali atoms with ns^1 electronic state $J = S = 1/2$

$$\mathbf{F} = \mathbf{J} + \mathbf{I}$$

^{87}Rb, ^{23}Na, ^{7}Li - $I = 3/2$: effective bosons

^{6}Li - $I = 1$, ^{40}K - $I = 4$: effective fermions

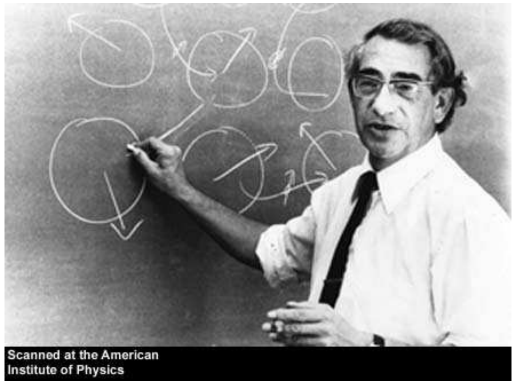


$$E_{int}^{solid} \sim 1 - 4eV \sim 10^4 K, \quad E_{kin}^{solid} \sim 1 - 10eV \sim 10^5 K$$

$$E_{kin}^{optical} \sim E_{int}^{optical} \sim 10kHz \sim 10^{-6} K$$

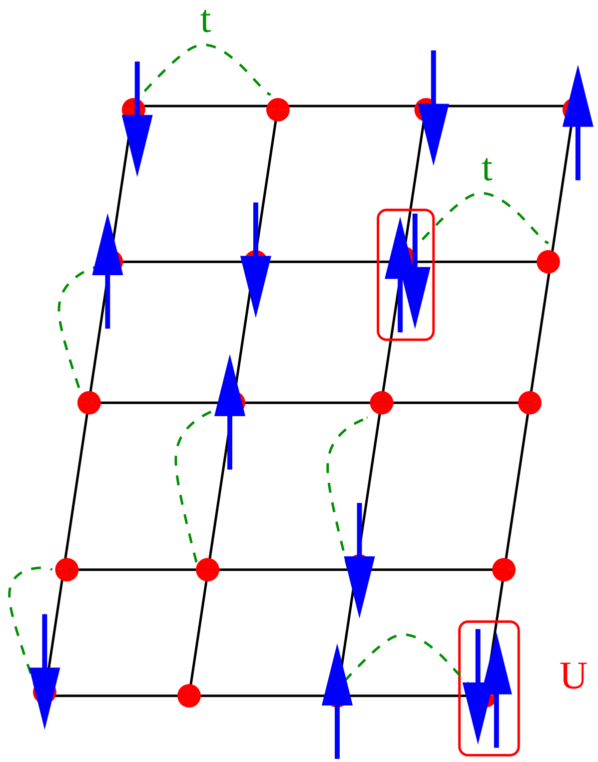
Correlated fermions on crystal and optical lattices

$$H = -\sum_{ij\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

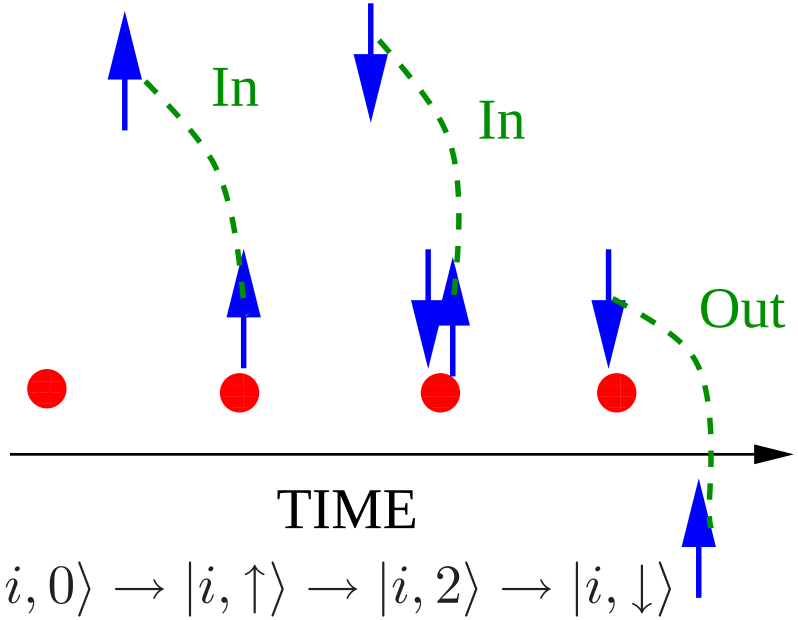


fermionic Hubbard model

P.W. Anderson, J. Hubbard, M. Gutzwiller, J. Kanamori, 1960-63



Local Hubbard physics

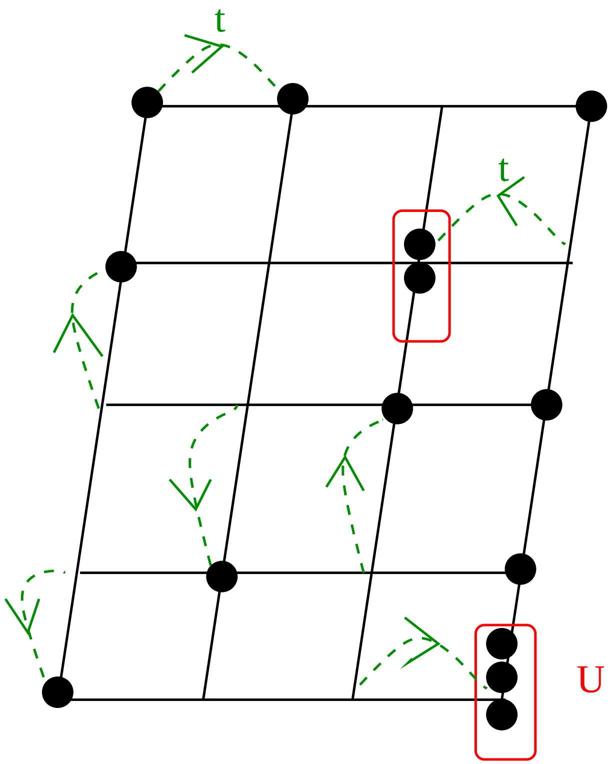


Correlated bosons on optical lattices

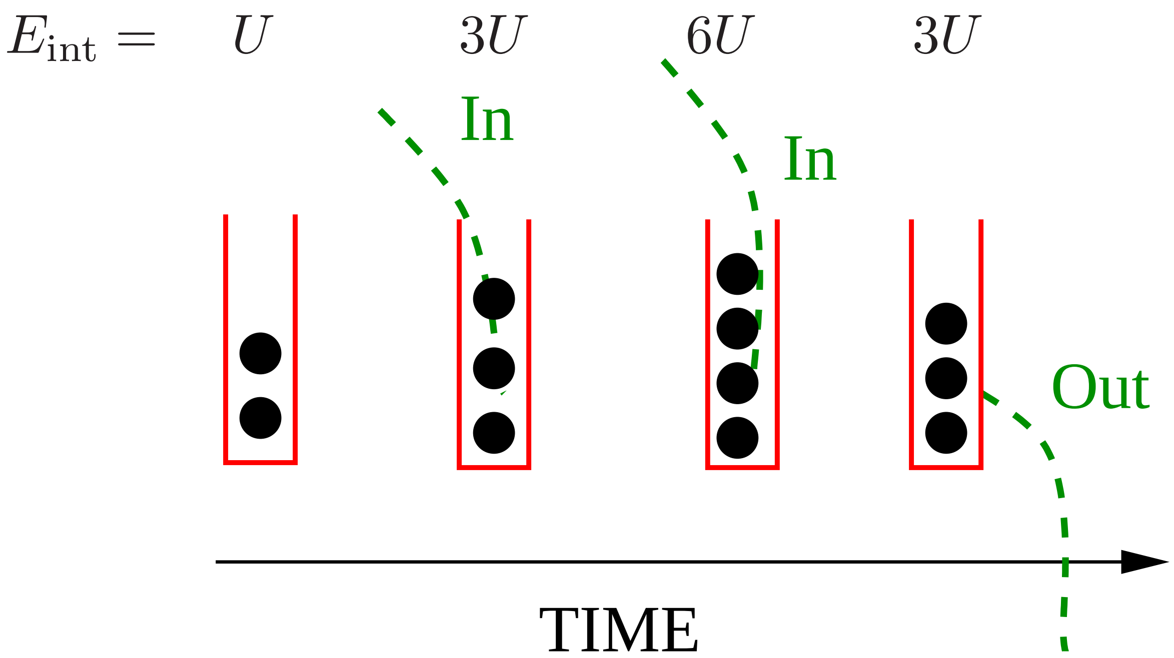
Gersch, Knollman, 1963
Fisher et al., 1989
Scalettar, Kampf, et al., 1995
Jacksch, 1998

bosonic Hubbard model

$$H = \sum_{ij} t_{ij}\, b_i^\dagger b_j + \frac{U}{2} \sum_i n_i (n_i - 1)$$



local (on-site) correlations in time



$$|i,2\rangle \to |i,3\rangle \to |i,4\rangle \to |i,3\rangle$$

integer occupation of single site changes in time

Origin of genuine many-body correlation

$$H = H^{\mathrm{hopping}} + H_{\mathrm{loc}}^{\mathrm{interaction}}$$

$$\left[H^{\mathrm{hopping}}, H_{\mathrm{loc}}^{\mathrm{interaction}}\right] \neq 0$$

How to solve Hubbard models?

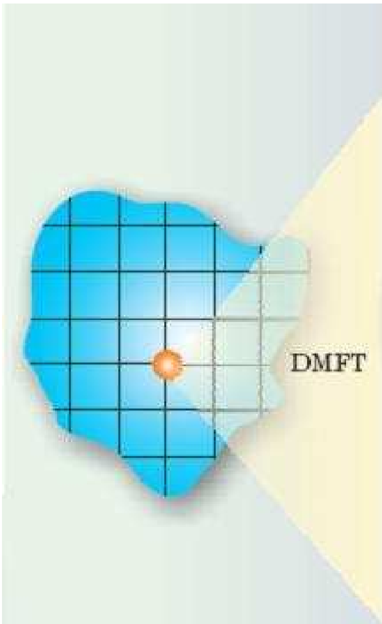
Dynamical Mean-Field Theory (DMFT)

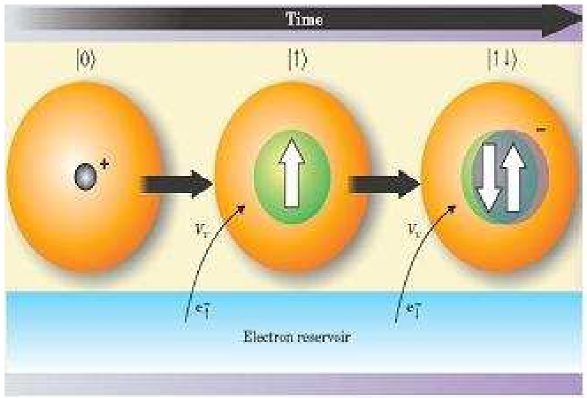
$$H = H^{\text{hopping}} + H^{\text{interaction}}_{\text{loc}}$$

- comprehensive (all input parameters, all temperatures, all phases, ...)
- thermodynamically consistent and conserving
- exact solution in the large dimensions (coordination number) limit
- keeps $\langle [H^{\text{hopping}}, H^{\text{interaction}}_{\text{loc}}] \rangle \neq 0$ to describe correlations

DMFT for lattice fermions

Replace (map) full many-body lattice problem by a single-site coupled to dynamical reservoir and solve such problem self-consistently





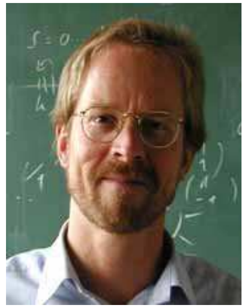
All local dynamical correlations included exactly

Space correlations neglected - mean-field approximation

DMFT scheme

S_{loc} - local interactions U or J from a model **TB** or a microscopic **LDA** Hamiltonian

D. Vollhardt



W. Metzner

$$\hat{G} = -\langle T\hat{C}(\tau)\hat{C}^*(0)\rangle_{S_{loc}}$$

DMFT

$$\hat{\mathcal{G}}^{-1} = \hat{G}^{-1} + \hat{\Sigma} \qquad \hat{\Sigma} \qquad \hat{\Sigma} = \hat{\mathcal{G}}^{-1} - \hat{G}^{-1}$$

G. Kotliar

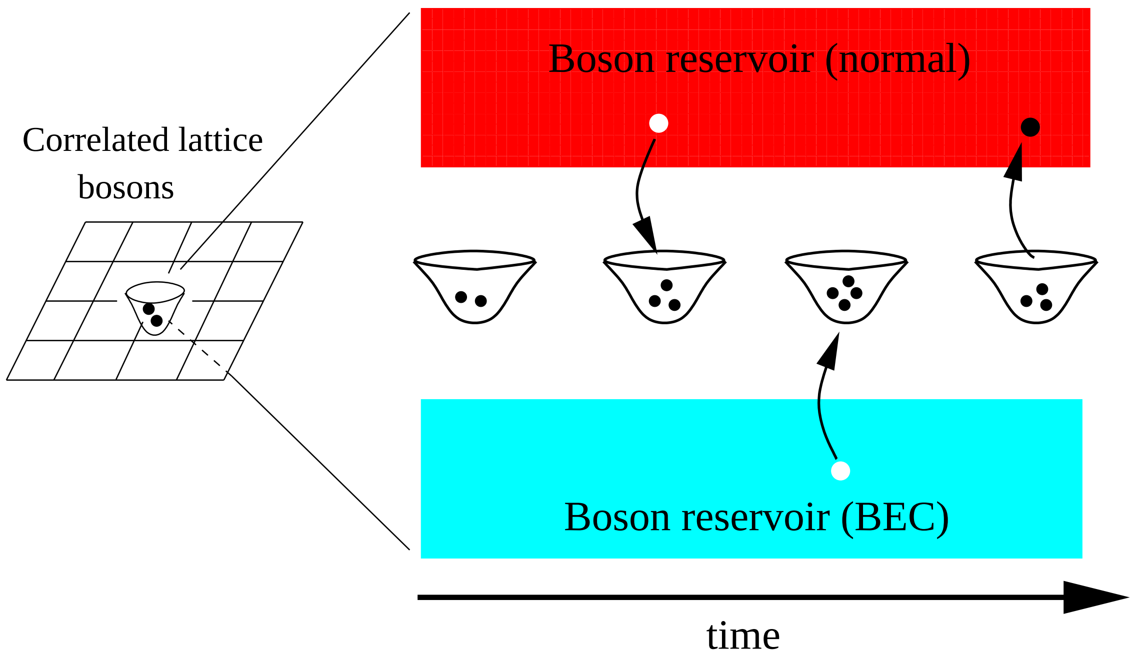
A. Georges

$$\hat{G} = \sum[(\omega+\mu)\hat{1} - \hat{H}^0 - \hat{\Sigma}]^{-1}$$

$\hat{H}^0$ is a model **TB** or a microscopic **LDA** Hamiltonian

Bosonic-Dynamical Mean-Field Theory (B-DMFT)

- Exact mapping of the lattice bosons in infinite dimension onto a single site
- Single site coupled to two reservoirs: normal bosons and bosons in the condensate
- Reservoirs properties are determined self-consistently, local correlations kept

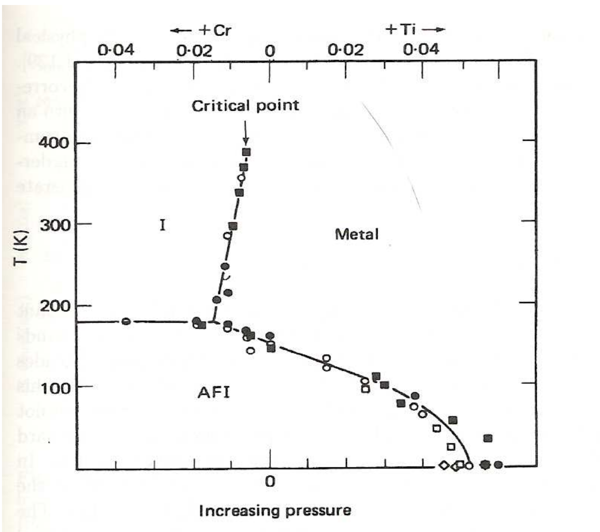


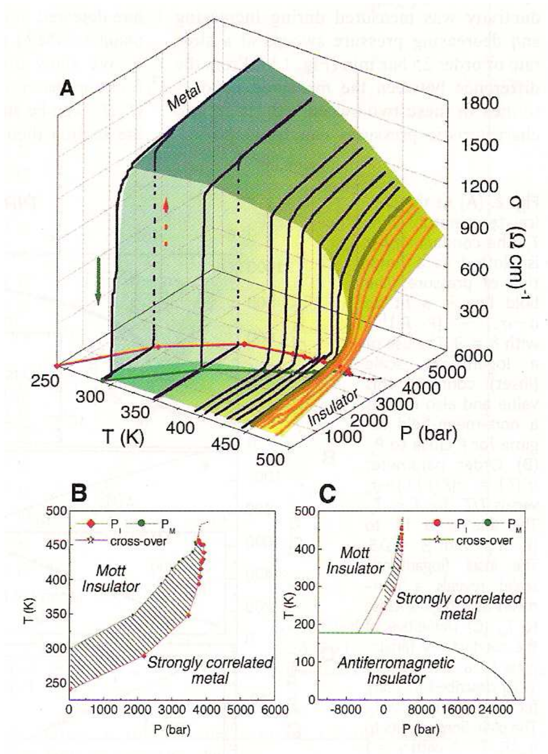
K.B., D. Vollhardt

Phys. Rev. B 77, 235106 (2008)

Mott-Hubbard metal insulator transition: V_2O_3

V $([Ar]3d^2 4s^2)$ gives V^{+3} valence band partially filled (metallic?)



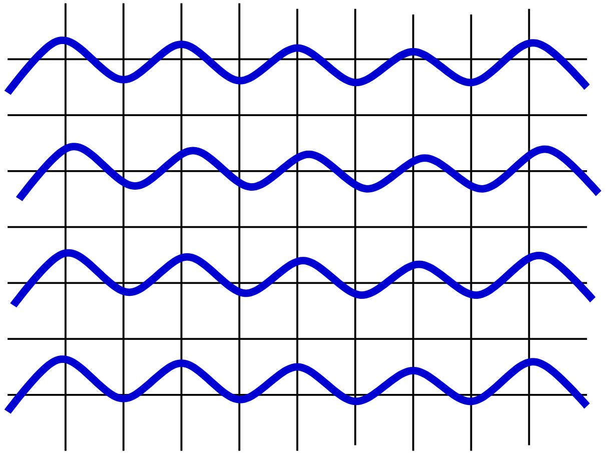


True Mott insulator

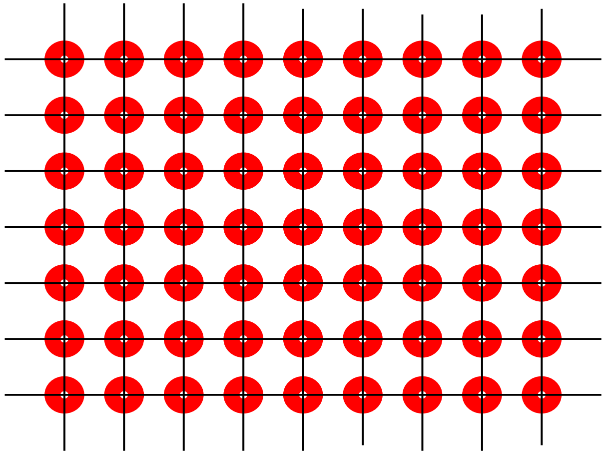
persists above T_N

Mott – Hubbard Insulator, Mott – Heisenberg Insulator, and Slater Insulator

MIT at half-filling

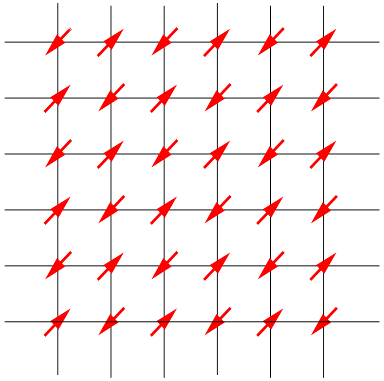


$U \ll |t_{ij}|$, $\Delta\mathbf{p} = 0$



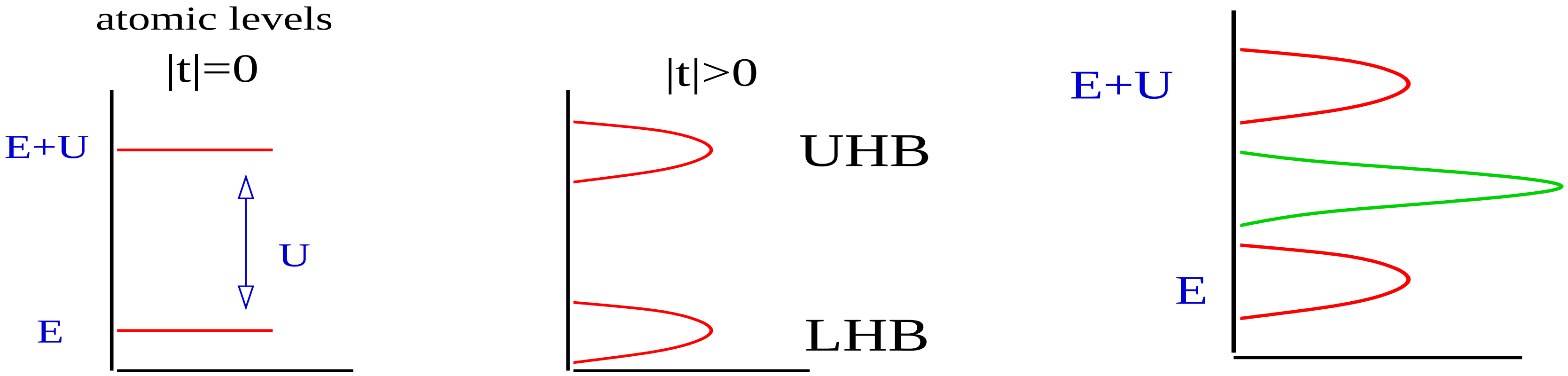
$U \gg |t_{ij}|$, $\Delta\mathbf{r} = 0$

Antiferromagnetic Mott insulator



typical intermediate coupling problem $U_c \approx |t_{ij}|$

MIT at half-filling



spin flip on central site

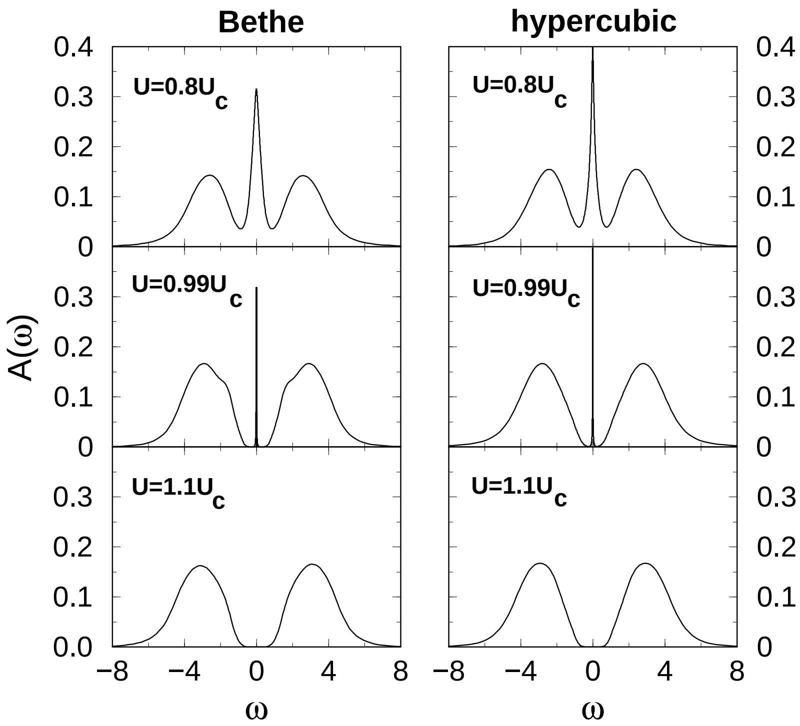
at $U = U_c$ resonance disapears

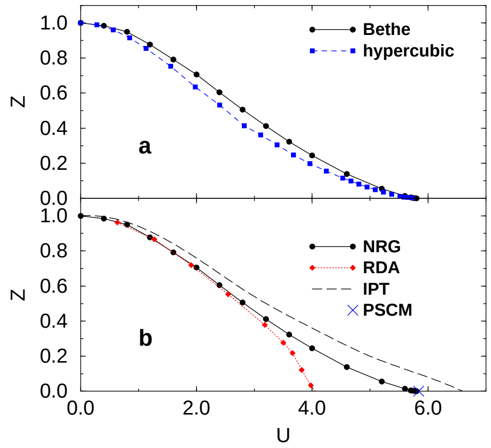
gaped insulator

dynamical processes with spin-flips inject states into correlation gap giving a quasiparticle resonance

MIT at half-filling at $T = 0$ according to DMFT

Kotliar et al. 92-96, Bulla, 99





Luttinger theorem $A(0) = N_0(0)$

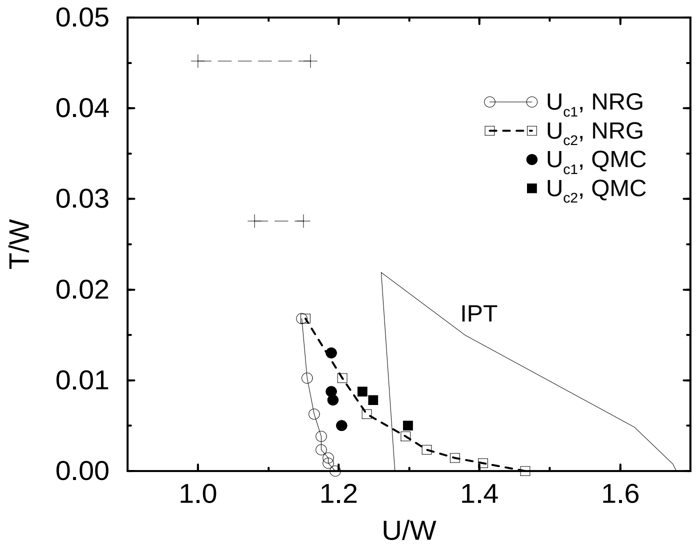
Fermi liquid

$$G(k,\omega) \sim \frac{Z}{\omega - \tilde{\epsilon}_k - i\alpha\ \omega^2} + G_{inc}$$

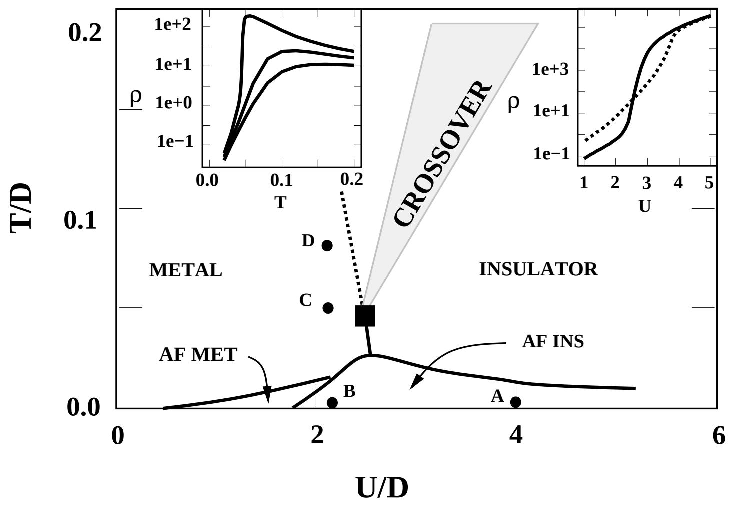
Muller-Hartmann 1989

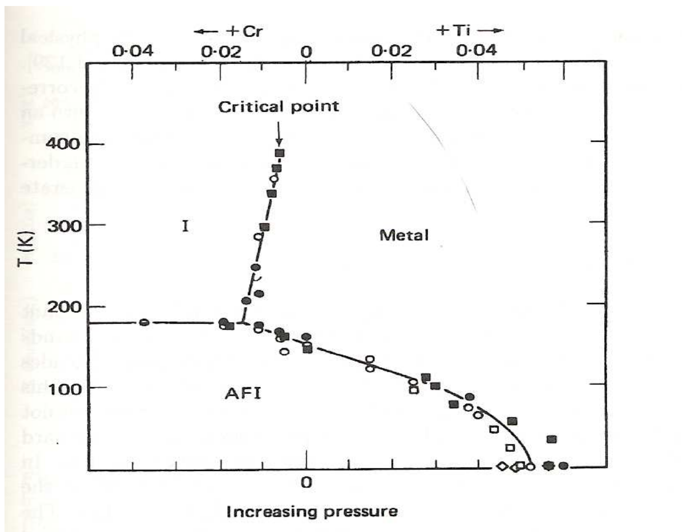
MIT at half-filling at $T > 0$ according to DMFT

Kotliar et al. 92-96, Bulla et al. 01, also Spalek 87



1^{st}-order transition





Correlation seen in dispersion of correlated electrons

One-particle spectral function - excitations at $\mathbf{k}$ and ω

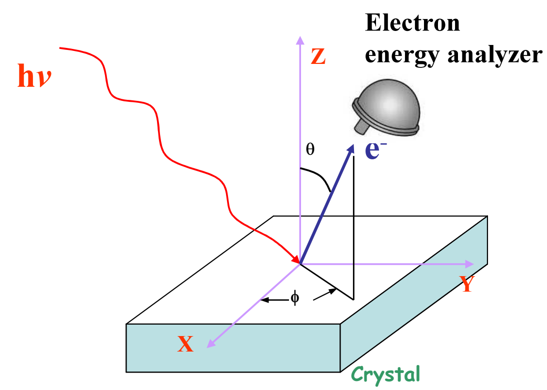
$$A(\mathbf{k},\omega) = -\frac{1}{\pi}\mathrm{Im}\frac{1}{\omega + \mu - \epsilon_{\mathbf{k}} - \Sigma(\mathbf{k},\omega)}$$

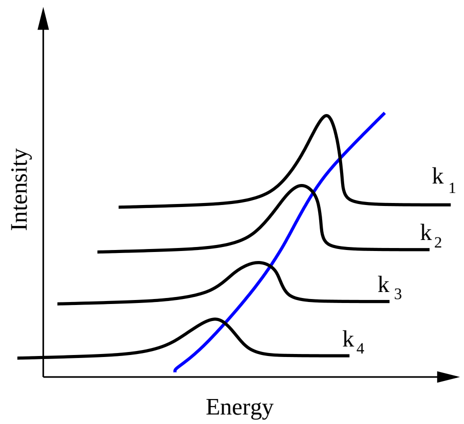
Dispersion relation $E_{\mathbf{k}}$

$$E_{\mathbf{k}} = \{\omega \text{ where } A(\mathbf{k},\omega) = \max\}$$

Dispersion relation is experimentally measured

Angular Resolved Photoemission Spectroscopy



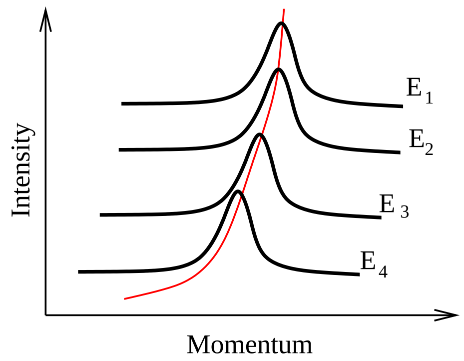


energy distribution curve (EDC)

$$k_x = k \cos\phi$$
$$k_y = k \sin\phi$$

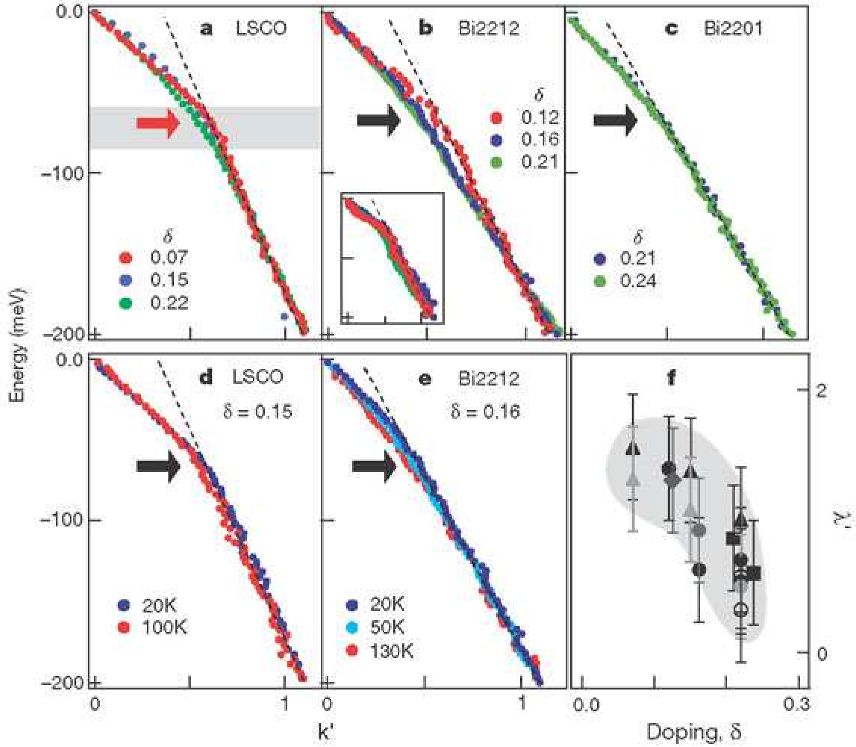
$$E = k^2/2m$$

energy resolution 1meV



momentum distribution curve (MDC)

Kinks in HTC

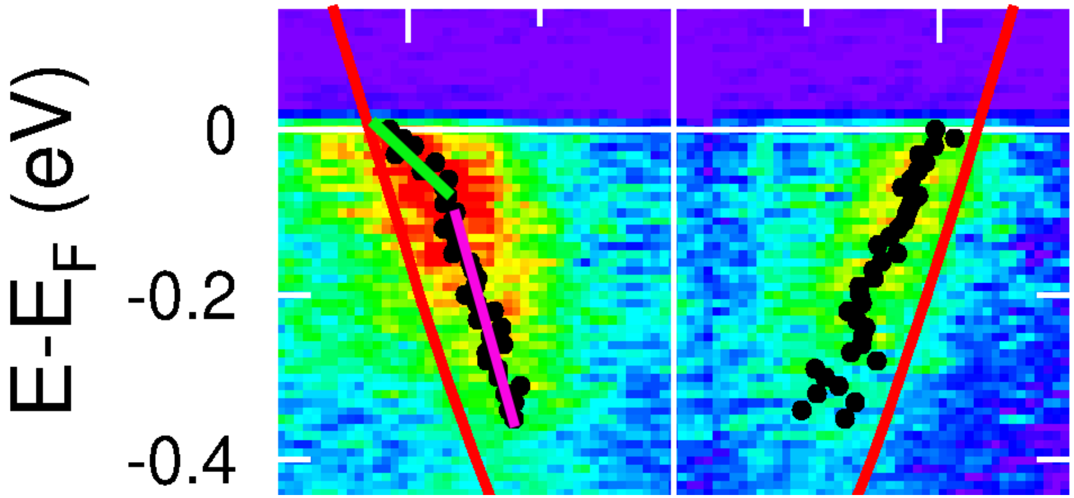


cond-mat/0604284

Kinks at $40 - 70$meV

electron-phonon or electron-spin fluctuations coupling

More examples of kinks in ARPES



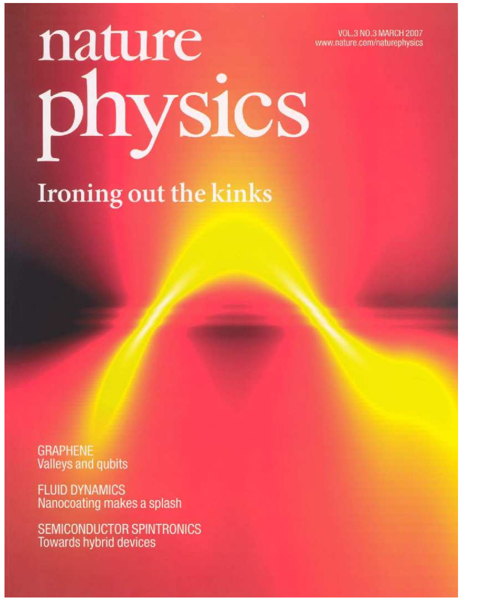
$SrVO_3$, cond-mat/0504075

Kinks seen experimentally at 150 meV

Pure electronic origin?

New purely electronic mechanism

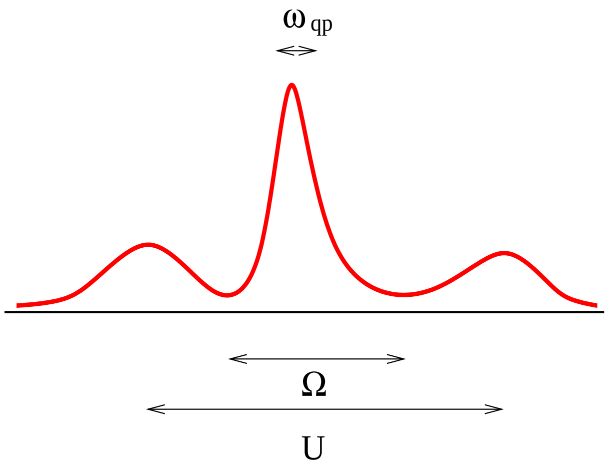
- in strongly correlated systems
- characteristic energy scale
- range of validity for Fermi liquid theory

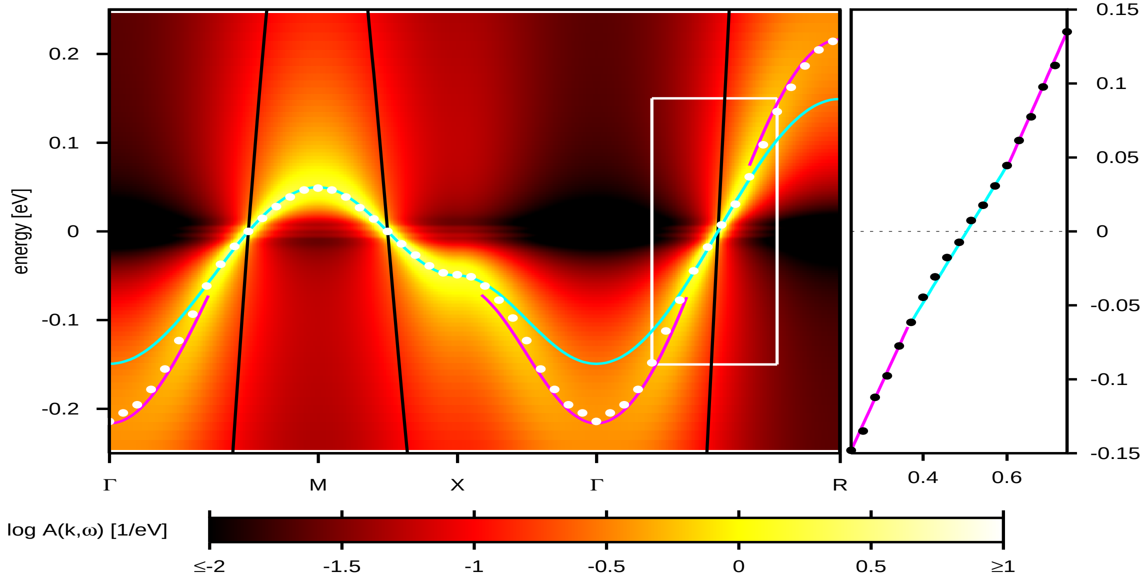


K.B., M. Kollar, K. Held, Y.-F. Yang, I. A. Nekrasov, Th. Pruschke, D. Vollhardt

Nature Physics 3, 168 (2007)

Kinks due to strong correlations





Fermi liquid $Z_{FL} \ll 1$: $E_{\mathbf{k}} = Z_{FL}\epsilon_{\mathbf{k}}$ for $|E_{\mathbf{k}}| < \omega_*$

Different renormalization $Z_{CP} \ll 1$: $E_{\mathbf{k}} = Z_{CP}\epsilon_{\mathbf{k}} \pm c$ for $|E_{\mathbf{k}}| > \omega_*$

Microscopic predictions

- Kink position

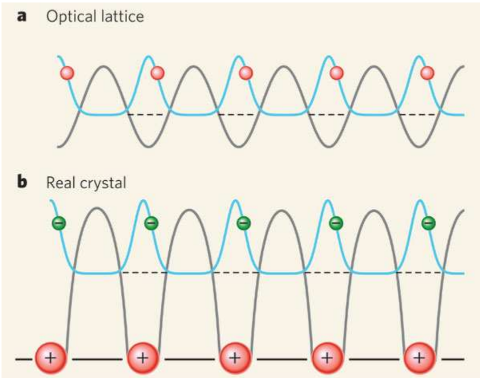
$$\omega_* = 0.41 Z_{FL} \frac{\mathrm{Im} 1/G_0}{\mathrm{Re} G_0'/G_0^2}$$

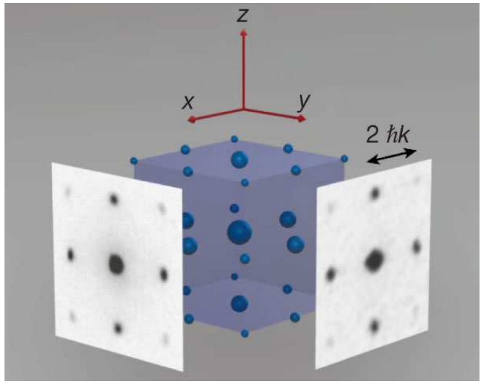
- Intermediate energy regime

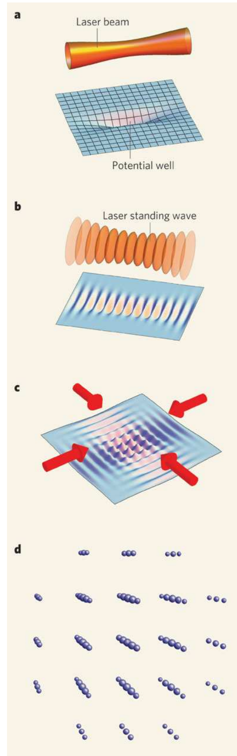
$$Z_{CP} = Z_{FL} \frac{1}{\mathrm{Re} G_0'/G_0^2}$$

- Change in the slope Z_{FL}/Z_{CP} interaction independent
- Curvature of the kink $\sim Z_{FL}^2$
- Sharpness of the kink $\sim 1/Z_{FL}^2$
- Sharper for stronger U

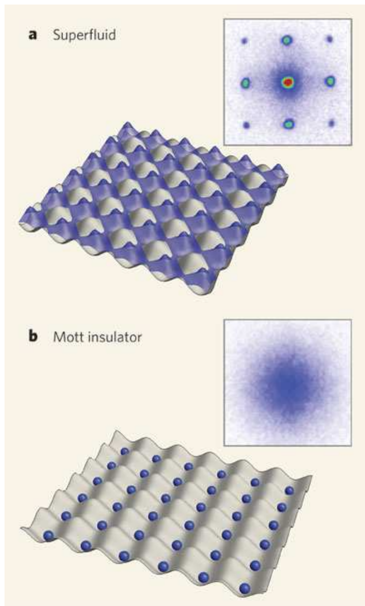
Superfluid-insulator transition in lattice bosons

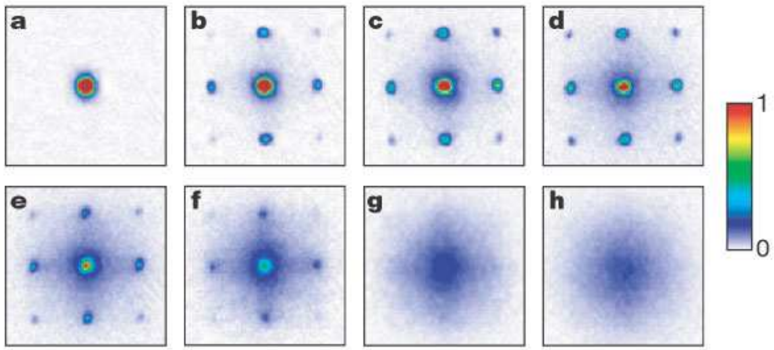






Optical lattices with cold atoms

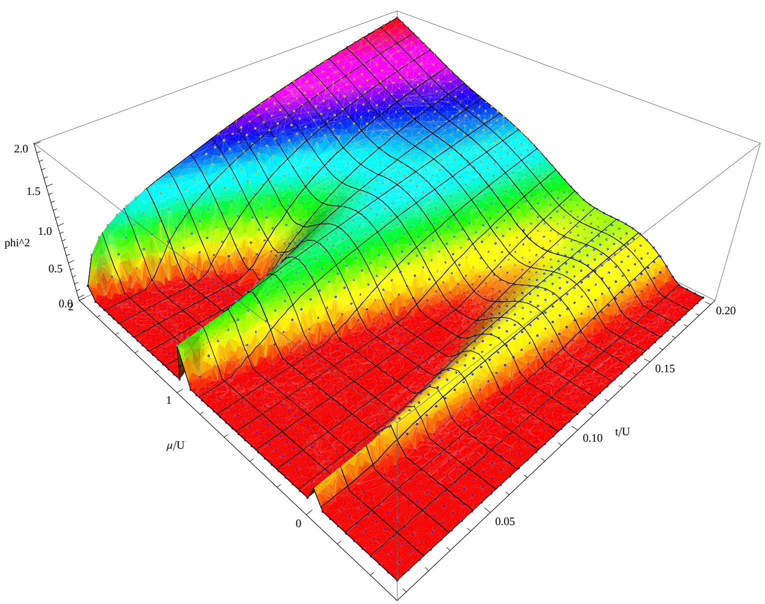




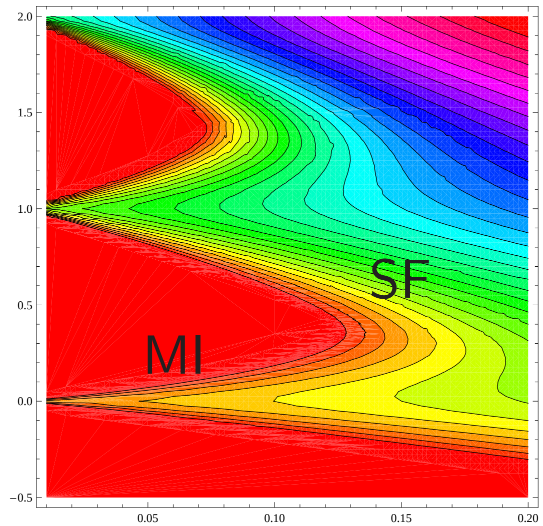
Superfluid-Mott insulator transition, Greiner, Mandel, Esslinger, Hänsch, Bloch, 2002

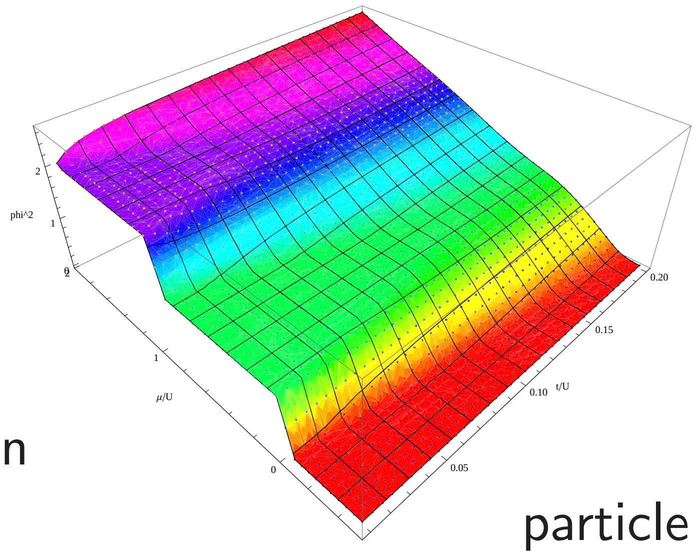
Bosonic Hubbard model: B-DMFT CT-QMC

Philipp Werner, Peter Anders: developed continous time Monte Carlo method for local (impurity) bosonic problem with B-DMFT self-consistency conditions



condensate density





particle density

Exact result for SF-Mott Insulator transition

Bethe DOS, $W = 4$, $\beta = 4$

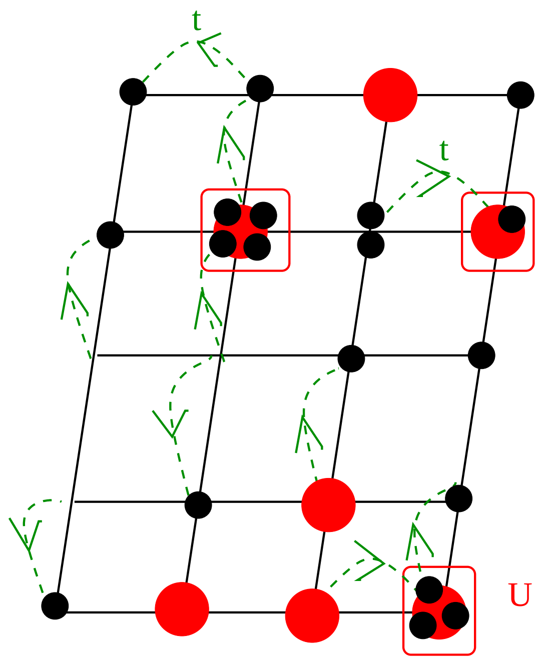
Bosonic Falicov-Kimball model

Binary mixture of itinerant (b) and localized (f) bosons on the lattice

$$H = \sum_{ij} t_{ij}\, b_i^\dagger b_j + \epsilon_f \sum_i f_i^\dagger f_i + U_{bf} \sum_i n_{bi} n_{fi} + U_{ff} \sum_i n_{fi} n_{fi}$$

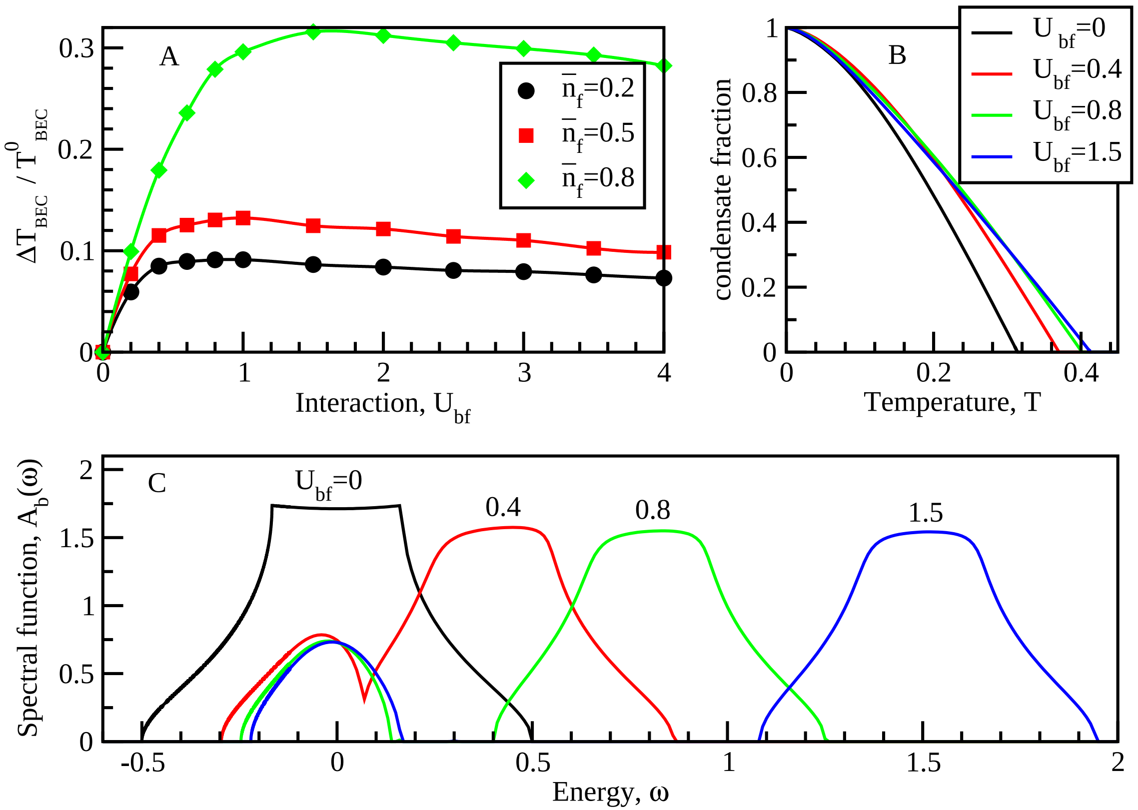
Local conservation law $[n_{fi}, H] = 0$ hence $n_{fi} = 0, 1, 2, \ldots$ classical variable

B-DMFT: local action Gaussian and analytically integrable



Enhancement of T_{BEC} due to interaction

Hard-core f-bosons $U_{ff} = \infty$; $n_f = 0, 1$; $0 \leq \bar{n}_f \leq 1$; $d = 3$ - SC lattice



KB, Vollhardt, PRB (2008)

$$A_b(\omega) = -\mathrm{Im} G_b(\omega)/\pi$$

$$\bar{n}_b = \bar{n}_b^{BEC} + \int d\omega \, \frac{A_b(\omega+\mu_b)}{e^{\omega/T} - 1}$$

Normal part decreases when U increases for constant μ_b and T

Quantifying correlations

How many correlation is there
in correlated electron systems?

We need information theory tools to address this issue.

Classical vs. Quantum Information Theory

Probability distribution vs. Density operator

$$p_k \longleftrightarrow \hat{\rho} = \sum_k p_k |k\rangle\langle k|$$

Shannon entropy vs. von Neumann entropy

$$I = -\langle \log_2 p_k \rangle = -\sum_k p_k \log_2 p_k \longleftrightarrow S = -\langle \ln \hat{\rho} \rangle = -Tr[\hat{\rho} \ln \hat{\rho}]$$

Two correlated (sub)systems have relative entropy

$$I = I_1 + I_2 - \Delta I \longleftrightarrow S = S_1 + S_2 - E$$

$$\Delta I(p_{kl}||p_k p_l) = -\sum_{kl} p_{kl}[\log_2 \frac{p_{kl}}{p_k p_l}] \longleftrightarrow E(\hat{\rho}||\hat{\rho}_1 \otimes \hat{\rho}_2) = -Tr[\hat{\rho}(\ln \hat{\rho} - \ln \hat{\rho}_1 \otimes \hat{\rho}_2)]$$

Relative entropy vanishes in the absence of correlations (product states)

Asymptotic distiguishability

Quantum Sanov theorem:
Probability P_n that a state $\hat{\sigma}$ is not distiguishable from a state $\hat{\rho}$ in n measurements, when $n \gg 1$, is

$$P_n \approx e^{-nE(\hat{\rho}||\hat{\sigma})}.$$

Relative entropy $E(\hat{\rho}||\hat{\sigma})$ as a 'distance' between quantum states.

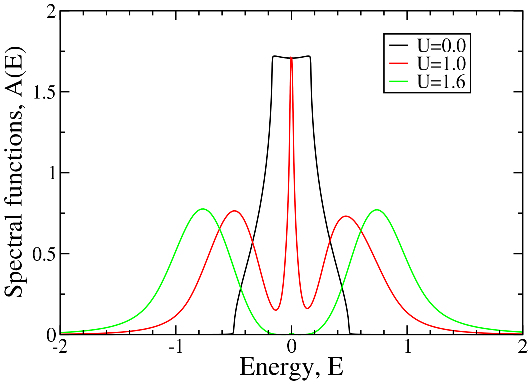
We calculate

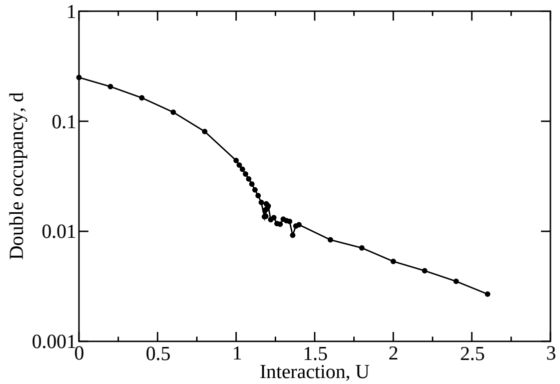
- von Neumann entropies and
- relative entropies

for and between different correlated and uncorrelated (product) states of the Hubbard model.

Correlation and Mott Transition

$$S(\hat\rho) = -Tr[\hat\rho \ln \hat\rho]$$
$$E(\hat\rho||\hat\sigma) = -Tr[\hat\rho \ln \hat\rho - \hat\rho \ln \hat\sigma]$$





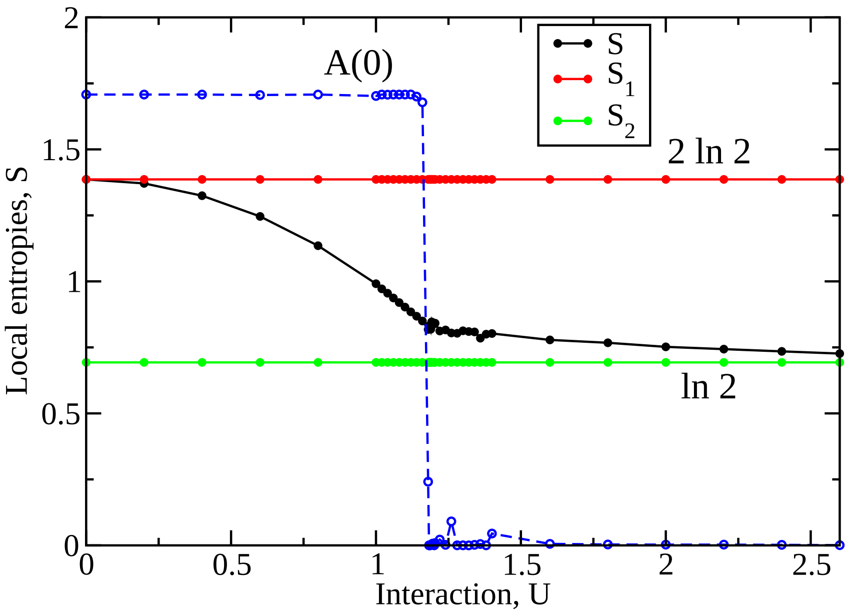
$$S = S(\hat\rho_{DMFT})$$
$$S_1 = S(\hat\rho_0)$$
$$S_2 = S(\hat\rho_a)$$

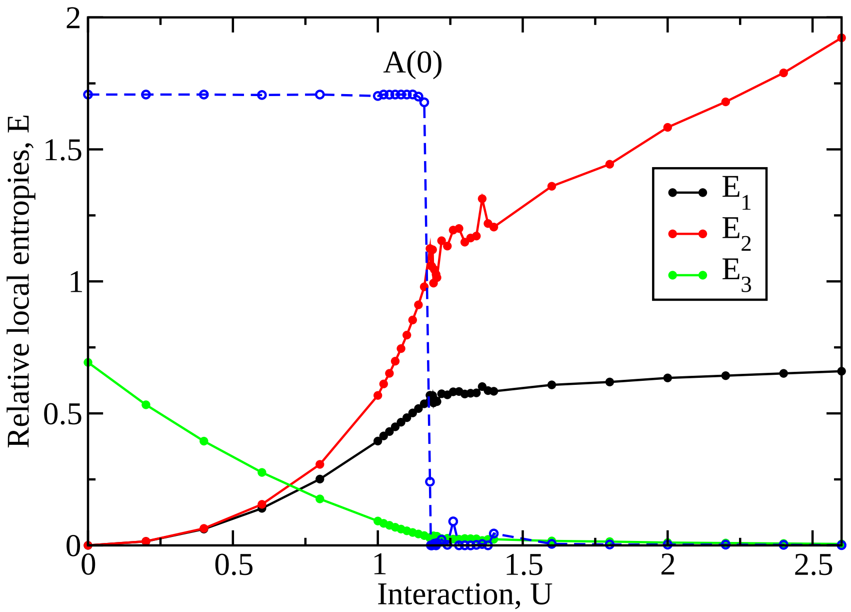
Product (HF) states:

$|0\rangle = \prod_{k\sigma}^{k_F} a_{k\sigma}^\dagger |v\rangle$ - $U = 0$ limit

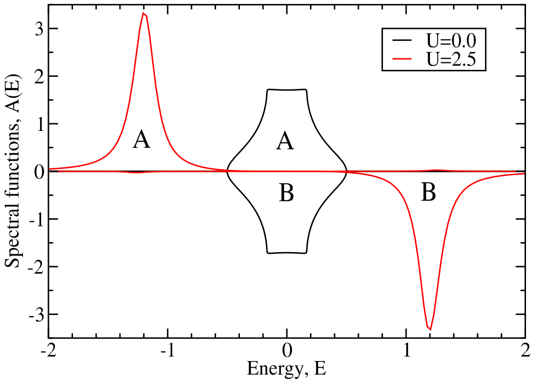
$|a\rangle = \prod_{i}^{N_L} a_{i\sigma_i}^\dagger |v\rangle$ - atomic limit

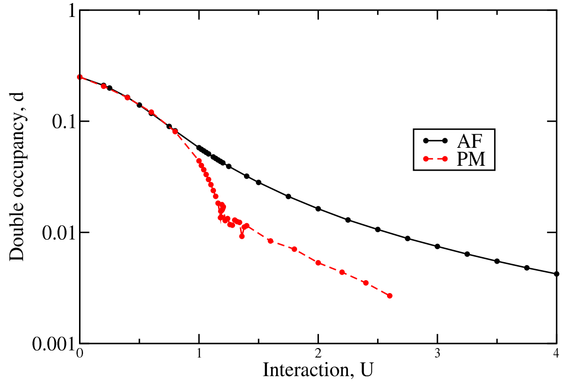
$$E_1 = E(\hat\rho_{DMFT}||\hat\rho_0)$$
$$E_2 = E(\hat\rho_0||\hat\rho_{DMFT})$$
$$E_3 = E(\hat\rho_a||\hat\rho_{DMFT})$$





Correlation and Antiferromagnetic Order





$$S(\hat{\rho}) = -Tr[\hat{\rho}\ln\hat{\rho}]$$

$$E(\hat{\rho}||\hat{\sigma}) = -Tr[\hat{\rho}\ln\hat{\rho} - \hat{\rho}\ln\hat{\sigma}]$$

$$S = S(\hat{\rho}_{DMFT})$$

$$S_1 = S(\hat{\rho}_0)$$

$$S_2 = S(\hat{\rho}_a)$$

Product (HF) states:

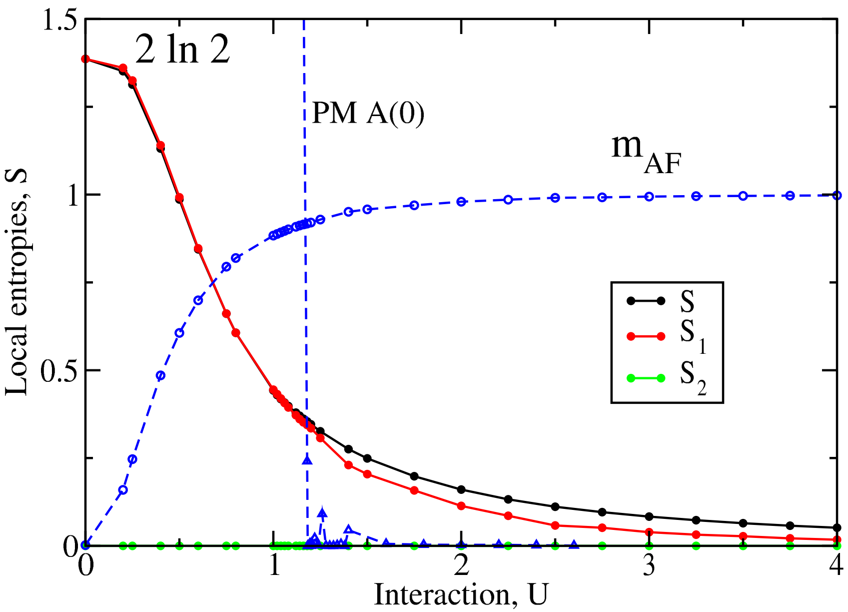
$|0\rangle = \prod_{k\in(A,B)}^{k_F} a^\dagger_{k_A\uparrow} a^\dagger_{k_B\downarrow}|v\rangle$ - Slater limit

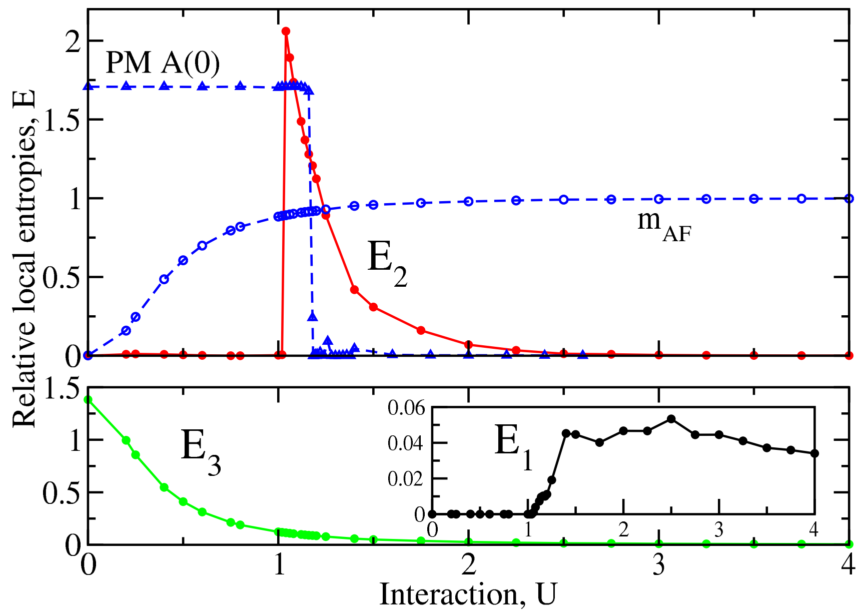
$|a\rangle = \prod_{i\in(A,B)}^{N_L} a^\dagger_{i_A\uparrow} a^\dagger_{i_B\downarrow}|v\rangle$ - Heisenberg limit

$$E_1 = E(\hat{\rho}_{DMFT}||\hat{\rho}_0)$$

$$E_2 = E(\hat{\rho}_0||\hat{\rho}_{DMFT})$$

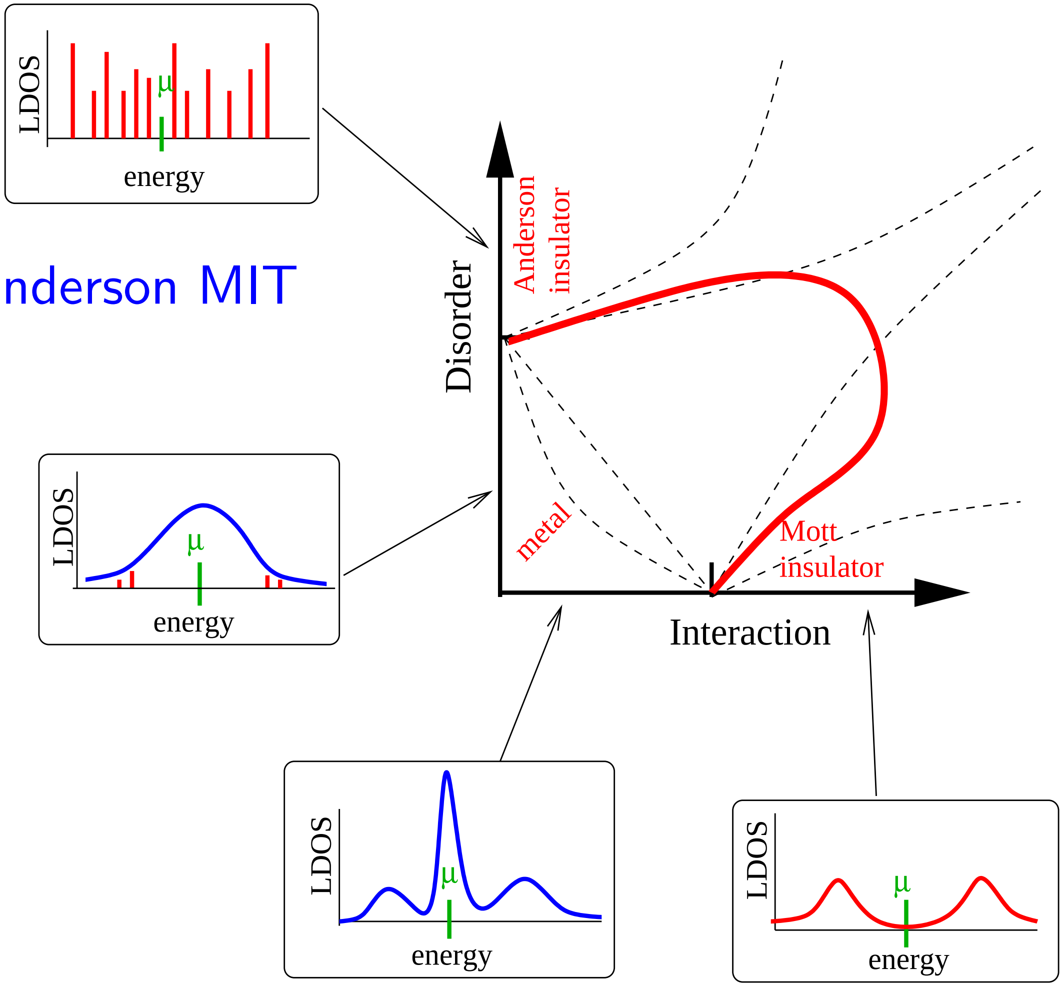
$$E_3 = E(\hat{\rho}_a||\hat{\rho}_{DMFT})$$





Disorder as a probe of correlations

Disorder ↔ Anderson MIT



Two insulators are
continously connected

BUT

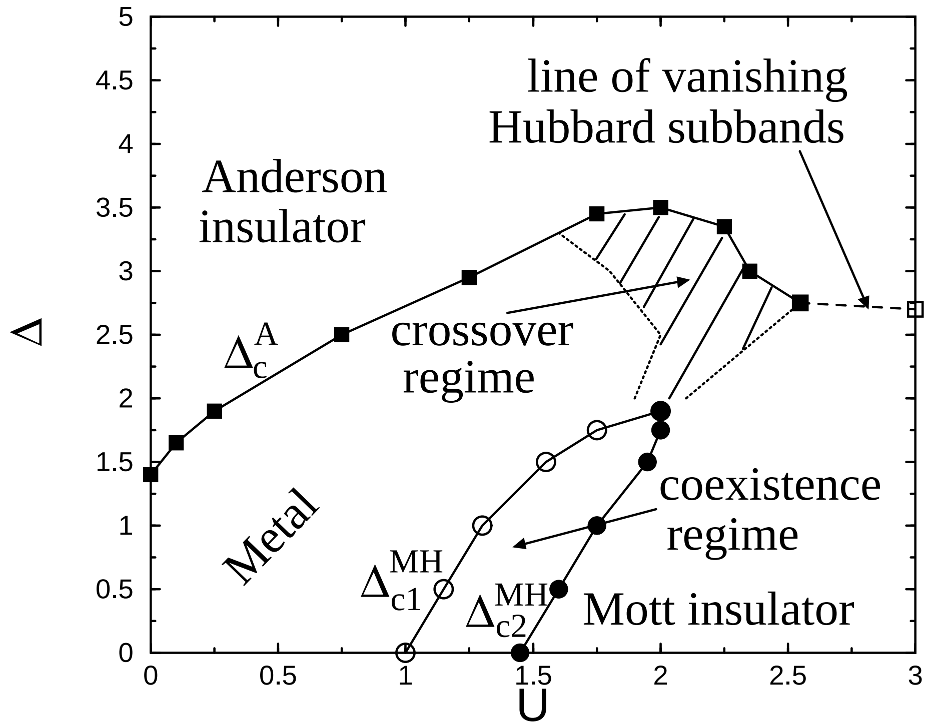
Interaction ↔ Mott-Hubbard MIT

Interaction and disorder compete with each other stabilizing the metallic phase against the occurring one of the insulators

Phase diagram for disordered Hubbard model

$$N_0(\epsilon) = \frac{2}{\pi D}\sqrt{D^2 - \epsilon^2}; \quad \eta(\omega) = \frac{D^2}{4} G(\omega)$$

$T = 0$, $n = 1$, $W = 2D = 1$, NRG solver



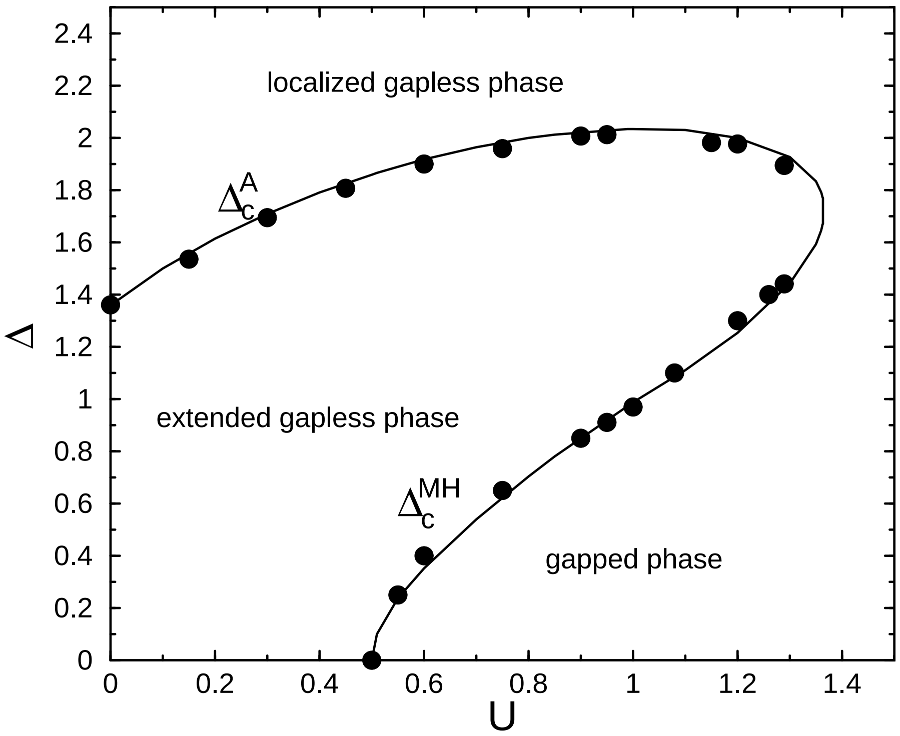
U - interaction, Δ - disorder

K.B. W. Hofstetter, D. Vollhardt, Phys. Rev. Lett. 94, 056404 (2005)

Phase diagram for disordered Falicov-Kimball model

$$H = \sum_{ij} t_{ij} c_i^\dagger c_j + \sum_i \epsilon_i c_i^\dagger c_i + U \sum_i c_i^\dagger c_i f_i^\dagger f_i$$

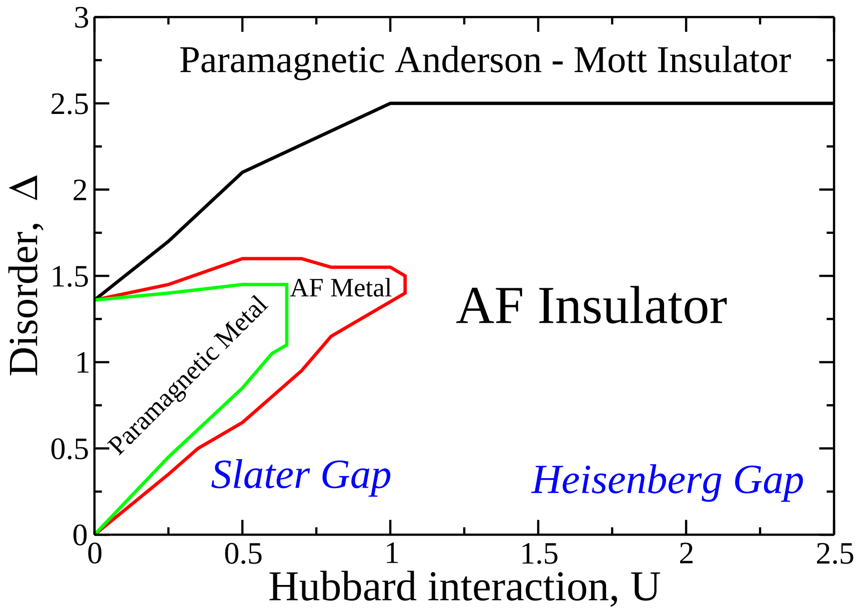
$T = 0$, $n = 1$, $W = 2D = 1$, analytical solver



U - interaction, Δ - disorder

K.B., Phys. Rev. B 71, 205105 (2005)

Mott-Anderson MIT with AF long-range order



No phase transition between Slater and Heisenberg limits

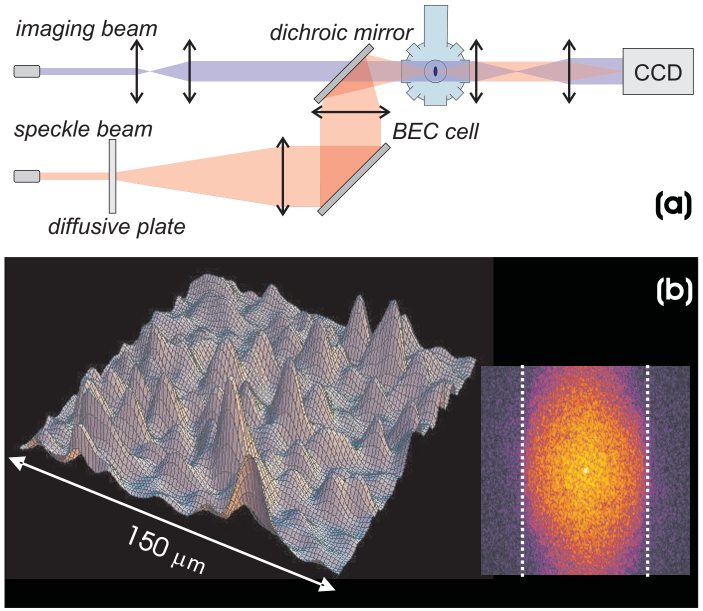
BUT

AF and PM metal only in Slater limit with disorder

K.B., W. Hofstetter, D. Vollhardt, Phys. Rev. Lett. 102, in press (2009)

Optical lattices with random disorder

- impurity atoms
- superposition of waves with different amplitudes (pseudo-random)
- speckle laser field on top of lattice (good random distribution)
- atom chips



$$H = J \sum_{ij} a^{\dagger}_{i\sigma} a_{j\sigma} + \sum_i \epsilon_i n_{i\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

Summary

- Correlation in many-body quantum physics

- Correlation is quantified by entropies

- Correlation is seen and tuned in solids and cold atoms
  - Mott-Hubbard metal-insulator transition
  - kinks in dispersions
  - superfluid-insulator transition
  - in phase diagrams when disorder is present

- Different correlations in paramagnetic and in antiferromagnetic cases