Correlated quantum particles in crystal and optical lattices

Krzysztof Byczuk

Institute of Theoretical Physics
Department of Physics
University of Warsaw

April 03rd, 2009
Collaboration

Dieter Vollhardt - Augsburg University

Walter Hofstetter - Frankfurt University
Marcus Kollar - Augsburg University
Anna Kauch - Augsburg University
Philipp Werner - ETH Zurich
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 10⁶) – 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 cured by (AF) long-range order ... but correlations are still missed
Correlated electrons

Narrow d, f-orbitals/bands → strong electronic correlations
Electronic bands in solids

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

Band insulators, e.g. NaCl

Atomic levels, localized electrons $| R_i \sigma \rangle$

Correlated metals, e.g. Ni, V$_2$O$_3$, Ce

Narrow bands, $| R_i \sigma \rangle \leftrightarrow | k \sigma \rangle$

Simple metals, e.g. Na, Al

Broad bands, extended Bloch waves $| k \sigma \rangle$
Electronic bands in solids

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

\[
\text{group velocity } v_k \approx \frac{\text{lattice spacing}}{\text{mean time}} = \frac{a}{\tau}
\]

Heisenberg principle $W \tau \sim \hbar$

\[
\frac{a}{\tau} \sim \frac{aW}{\hbar} \implies \tau \sim \frac{\hbar}{W}
\]

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 $a \sim 400 - 500 \text{nm}$

alkali atoms with $\text{ns}^1$ electronic state $J = S = 1/2$

$F = J + I$

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

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

dipol interaction - hopping

atom scattering - Hubbard $U$

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

$E_{\text{kin}}^{\text{optical}} \sim E_{\text{int}}^{\text{optical}} \sim 10k\text{Hz} \sim 10^{-6} K$
Correlated fermions on crystal and optical lattices

\[ H = - \sum_{ij\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} \]

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

Local Hubbard physics

\[ |i, 0\rangle \rightarrow |i, \uparrow\rangle \rightarrow |i, 2\rangle \rightarrow |i, \downarrow\rangle \]
Correlated bosons on optical lattices

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

\[ E_{\text{int}} = U \quad 3U \quad 6U \quad 3U \]

integer occupation of single site changes in time
Origin of genuine many-body correlation

\[ H = H^{\text{hopping}} + H^{\text{interaction}} \]

\[
\left[ H^{\text{hopping}}, H^{\text{interaction}} \right] \neq 0
\]
How to solve Hubbard models?

Dynamical Mean-Field Theory (DMFT)

\[ H = H^{\text{hopping}} + H^{\text{interaction}} \]

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

\[ S_{loc} - \text{local interactions } U \text{ or } J \text{ from a model TB or a microscopic LDA Hamiltonian} \]

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

\[ \hat{G}^{-1} = \hat{G}^{-1} + \hat{\Sigma} \]

\[ \hat{\Sigma} = \hat{G}^{-1} - \hat{G}^{-1} \]

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

\[ \hat{H}^0 \text{ is a model TB or a microscopic LDA Hamiltonian} \]
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
Mott-Hubbard metal insulator transition: $V_2O_3$

$V\ ([Ar]3d^24s^2)$ 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

\[ U \ll |t_{ij}|, \Delta p = 0 \]

\[ U \gg |t_{ij}|, \Delta r = 0 \]

Antiferromagnetic Mott insulator

typical intermediate coupling problem \( U_c \approx |t_{ij}| \)
MIT at half-filling

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

atomic levels

|t|=0

|t|>0

at \( U = U_c \) resonance disappears

gaped insulator

spin flip on central site
MIT at half-filling at $T = 0$ according to DMFT

Kotliar et al. 92-96, Bulla, 99

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

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

Fermi liquid

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\textsuperscript{st}-order transition
Correlation seen in dispersion of correlated electrons

One-particle spectral function - excitations at $k$ and $\omega$

$$A(k, \omega) = -\frac{1}{\pi} \text{Im} \frac{1}{\omega + \mu - \epsilon_k - \Sigma(k, \omega)}$$

Dispersion relation $E_k$

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

Dispersion relation is experimentally measured
Angular Resolved Photoemission Spectroscopy

Energy distribution curve (EDC)

\[ k_x = k \cos \phi \]
\[ k_y = k \sin \phi \]
\[ E = \frac{k^2}{2m} \]

energy resolution 1meV

momentum distribution curve (MDC)
Kinks in HTC

Kinks at 40 – 70 meV

electron-phonon or electron-spin fluctuations coupling

cond-mat/0604284
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
Kinks due to strong correlations

Fermi liquid $Z_{FL} \ll 1$: $E_k = Z_{FL}\epsilon_k$ for $|E_k| < \omega_*$

Different renormalization $Z_{CP} \ll 1$: $E_k = Z_{CP}\epsilon_k \pm c$ for $|E_k| > \omega_*$
Microscopic predictions

• Kink position

\[ \omega_* = 0.41 \frac{Z_{FL}}{Z_{CP}} \frac{\text{Im}1/G_0}{\text{Re}G_0'}/G_0^2 \]

• Intermediate energy regime

\[ Z_{CP} = Z_{FL} \frac{1}{\text{Re}G_0'}/G_0^2 \]

• 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,
**Bosonic Hubbard model: B-DMFT CT-QMC**

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

![Diagram](attachment:image.png)

condensate density

Exact result for SF-Mott Insulator transition

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

particle density
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

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

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

Normal part decreases when $U$ increases for constant $\mu_b$ 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

\[ p_k \leftrightarrow \hat{\rho} = \sum_k p_k |k\rangle\langle k| \]

Shannon entropy vs. von Neumann entropy

\[ I = -\left< \log_2 p_k \right> = -\sum_k p_k \log_2 p_k \leftrightarrow S = -\left< \ln \hat{\rho} \right> = -Tr[\hat{\rho} \ln \hat{\rho}] \]

Two correlated (sub)systems have relative entropy

\[ I = I_1 + I_2 - \Delta I \leftrightarrow S = S_1 + S_2 - E \]

\[ \Delta I(p_{kl}||p_{kp'l}) = -\sum_{kl} p_{kl} \left[ \log_2 \frac{p_{kl}}{p_{kp'l}} \right] \leftrightarrow E(\hat{\rho}||\hat{\rho}_1 \otimes \hat{\rho}_2) = -Tr[\hat{\rho} (\ln \hat{\rho} - \ln \hat{\rho}_1 \otimes \hat{\rho}_2)] \]

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

Quantum Sanov theorem:
Probability $P_n$ that a state $\hat{\sigma}$ is not distinguishable 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

\[ S(\hat{\rho}) = -T r[\hat{\rho} \ln \hat{\rho}] \]
\[ E(\hat{\rho}||\hat{\sigma}) = -T r[\hat{\rho} \ln \hat{\rho} - \hat{\rho} \ln \hat{\sigma}] \]

\[ S = S(\hat{\rho}_{DMFT}) \]
\[ S_1 = S(\hat{\rho}_0) \]
\[ S_2 = S(\hat{\rho}_1) \]

Product (HF) states:
\[ |0\rangle = \prod_{k\sigma}^{k_F} a_{k\sigma}^\dagger |v\rangle - \text{U} = 0 \text{ limit} \]
\[ |a\rangle = \prod_{i\sigma_i}^{N_L} a_{i\sigma_i}^\dagger |v\rangle - \text{atomic limit} \]
Correlation and Antiferromagnetic Order

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

\[ S = S(\hat{\rho}_{DMFT}) \]
\[ S_1 = S(\hat{\rho}_0) \]
\[ S_2 = S(\hat{\rho}_a) \]

Product (HF) states:

\[ |0\rangle = \prod_{k \in (A,B)}^{k_F} a_{kA}^\dagger \sigma_{kB} \langle \nu | \] - Slater limit
\[ |a\rangle = \prod_{i \in (A,B)}^{N_L} a_{iA}^\dagger \sigma_{iB} \langle \nu | \] - Heisenberg limit

---

Local entropies, \( S \)

\[ \text{Interaction, } U \]

Relative local entropies, \( E \)

\[ \text{Interaction, } U \]
Disorder as a probe of correlations

Two insulators are continuously connected

BUT

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

Phase diagram for disordered Falicov-Kimball model

\[ H = \sum_{i,j} t_{ij} c_i^\dagger c_j + \sum_i \epsilon_i c_i^\dagger c_i + U \sum_i c_i^\dagger c_i f_i^\dagger f_i \]

\[ T = 0, \quad n = 1, \quad W = 2D = 1, \quad \text{analytical solver} \]

\[ U - \text{interaction}, \quad \Delta - \text{disorder} \]

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

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

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