Surprising Effects of Electronic Correlations in Solids

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Outline:

- Peculiarities of many-particle systems
- Correlations
- Electronic correlations in solids
- Dynamical Mean-Field Theory: Models vs. materials
- New Developments & Perspectives
Peculiarities of Many-Particle Systems
Interacting many-particle systems

Elementary ("bare") particles + fundamental interactions

\[ N \rightarrow \infty \]

effective ("quasi") particles + effective interactions

\[ \frac{Q}{r} \]

Vacuum

Coulomb potential
Interacting many-particle systems

Elementary ("bare") particles + fundamental interactions

\[ N \to \infty \]

effective ("quasi") particles + effective interactions

Electron gas: Screening
Simplest approximation: Thomas-Fermi

Effective Yukawa potential
Interacting many-particle systems

Elementary ("bare") particles + fundamental interactions

\[ N \rightarrow \infty \]

effective ("quasi") particles + effective interactions

Electron gas: Screening
Better approximation: Lindhard

\[ \frac{Q}{r^3} \cos(2k_Fr) \]

Friedel oscillations
Interacting many-particle systems

Elementary ("bare") particles + fundamental interactions

\[ N \rightarrow \infty \]

effective ("quasi") particles + effective interactions

Electrons in solids

"Strong interaction" of electrons in localized orbitals
Quasiparticles
Bare electrons

\[ \text{Spin} = \frac{1}{2} \hbar \quad \text{Fermion} \]

\[ \downarrow \]

Fermi-Dirac statistics

\[ \downarrow \]

Pauli exclusion principle of many fermions

Fermi body/surface
Fermi gas: **Ground state**
Fermi gas: Excited states ($T>0$)

Switch on short range, repulsive interaction adiabatically ($d=3$)

Exact $k$-states ("particles"): infinite life time
Landau Fermi liquid

“Standard model of condensed matter physics“

Well-defined \( k \)-states ("quasiparticles") with
- finite life time
- effective mass
- effective interaction

\( \text{Fermi surface} \rightarrow \) (Quasi-) Particle
\( = \text{elementary excitation} \)

1-1 correspondence between one-particle states \( (k, \sigma) \)

Landau (1956/58)
Simple metals

**Potassium**

\[
\lim_{T \to 0} \frac{C_V}{T} = \gamma \propto \frac{m^*}{m}, \quad v_F = \frac{\hbar k_F}{m^*}
\]

Result of elementary excitations (quasiparticles)

"Heavy Fermions"

Steglich et al. (1979)

Stewart et al. (1983)

\( m^* \approx 1000 \ m \)

CeCu\(_2\)Si\(_2\), UBe\(_{13}\):

electrons interact strongly
Entirely new phenomena, e.g., phase transitions

Unpredicted “emergent” behavior

We used to think that if we knew one, we knew two, because one and one are two. We are finding out that we must learn a great deal more about 'and'.

Arthur Eddington (1882-1944)

“More is different” Anderson (1972)
Emergence

Examples:

- Superconductivity
- Magnetism
- Galaxy formation
- Traffic
- Weather
- Stock market
- Ants
- Human body
- Consciousness

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Correlations
Correlation [lat.]: con + relatio ("with relation")

Grammar: either ... or

Mathematics, natural sciences:

\[ \langle AB \rangle \neq \langle A \rangle \langle B \rangle \]

e.g., densities:

\[ \langle \rho(r)\rho(r') \rangle \neq \langle \rho(r) \rangle \langle \rho(r') \rangle \]

Assumption \[ \langle \rho(r)\rho(r') \rangle \approx \langle \rho(r) \rangle \langle \rho(r') \rangle \Rightarrow \]
Temporal/spatial correlations in everyday life

Correlations vs. long-range order
Correlations vs. long-range order

Sempe, THE NEW YORKER
Temporal/spatial correlations in everyday life
Temporal/spatial correlations in everyday life

Time/space average insufficient
Electronic Correlations in Solids
Partially filled d-orbitals

Partially filled f-orbitals

Narrow d,f-orbitals/bands → strong electronic correlations
Correlated electron materials

Fascinating topics for fundamental research

- large resistivity changes
- gigantic volume changes
- high-$T_c$ superconductivity
- strong thermoelectric response
- colossal magnetoresistance
- huge multiferroic effects

Technological applications:
- sensors, switches
- magnetic storage
- refrigerators
- functional materials, ...
Electronic Correlations: Models
The Hubbard model can be described by the Hamiltonian:

\[ H = -t \sum_{\langle i,j \rangle, \sigma} c_{i \sigma}^\dagger c_{j \sigma} + U \sum_i n_{i \uparrow} n_{i \downarrow} \]

- \( t \) is the hopping parameter.
- \( U \) is the on-site repulsion.
- \( n_{i \sigma} \) is the number operator for spin \( \sigma \) at site \( i \).

**References:**
- Gutzwiller, 1963
- Hubbard, 1963
- Kanamori, 1963
The Hubbard model is given by the Hamiltonian:

\[ H = -t \sum_{\langle i,j \rangle, \sigma} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} \]

where:
- \( H \) is the Hamiltonian.
- \( t \) is the hopping parameter.
- \( c_{i\sigma}^\dagger \) and \( c_{i\sigma} \) are creation and annihilation operators for an electron with spin \( \sigma \) at site \( i \).
- \( U \) is the on-site repulsion energy.
- \( n_{i\uparrow} \) and \( n_{i\downarrow} \) are the occupation numbers for spin-up and spin-down electrons at site \( i \).

This model was introduced by Gutzwiller in 1963, Hubbard in 1963, and Kanamori in 1963.
Central to the discussion is the Hubbard model, a theoretical framework for understanding quantum systems. The model is given by:

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

where $c_{i\sigma}^\dagger$ and $c_{i\sigma}$ are creation and annihilation operators, respectively, $t$ is the hopping integral, and $U$ is the on-site repulsion energy. The diagram illustrates the time evolution of the system.

**Theoretical challenge:**
Construct reliable, comprehensive non-perturbative approximation scheme.

**Notes:**
- Purely numerical approaches ($d=2,3$): hopeless.
- Static (Hartree-Fock-type) mean-field theories generally insufficient.

**Citations:**
- Gutzwiller, 1963
- Hubbard, 1963
- Kanamori, 1963
Dynamical Mean-Field Theory (DMFT) of Correlated Electrons
Theory of strongly correlated electrons

\[ H = -t \sum_{\langle i,j \rangle, \sigma} c_{i \sigma}^\dagger c_{j \sigma} + U \sum_i n_{i \uparrow} n_{i \downarrow} \quad \text{Hubbard model} \]

Face-centered cubic lattice

Dimension \(d=3\)

Face-centered cubic lattice with \(Z=12\)

\[ \sum(\omega) \]

\[ G(\omega) \]

“Dynamical (single-site) mean-field theory“

- Metzner, DV (1989)
- Müller-Hartmann (1989)
- Brandt and Mielsch (1989)
- Janis (1991)
- Georges and Kotliar (1992)
- Jarrell (1992)
Dynamical mean-field theory (DMFT) of correlated electrons

Proper time resolved treatment of local electronic interactions:

Georges, Kotliar (1992)

Physics Today
Kotliar, DV (2004)

“Spectral transfer”

Experimentally detectable?
Correlated Electron: Materials
<table>
<thead>
<tr>
<th>DFT/LDA</th>
<th>Model Hamiltonians</th>
</tr>
</thead>
<tbody>
<tr>
<td>+ material specific: “ab initio”</td>
<td>- input parameters unknown</td>
</tr>
<tr>
<td>- fails for strong correlations</td>
<td>+ systematic many-body approach</td>
</tr>
<tr>
<td>+ fast code packages</td>
<td>- computationally expensive</td>
</tr>
</tbody>
</table>

How to combine?

Held (2004)

time-averaged electron density
lattice potential
Computational scheme for correlated electron materials:

Material specific electronic structure
(Density functional theory: LDA, GGA, ... ) or GW

+ Local electronic correlations
(Many-body theory: DMFT)

LDA+DMFT

Anisimov, Poteryaev, Korotin, Anokhin, Kotliar (1997)
Lichtenstein, Katsnelson (1998)

Nekrasov, Held, Blümer, Poteryaev, Anisimov, DV (2000)
Computational scheme for correlated electron materials:

**Material specific electronic structure**
(Density functional theory: LDA, GGA, ...) or GW

**Local electronic correlations**
(Many-body theory: DMFT)

Held, Nekrasov, Keller, Eyert, Blümer, McMahan, Scalettar, Pruschke, Anisimov, DV (Psi-k 2003)
Application of LDA+DMFT

(Sr,Ca)VO$_3$: 3d$^1$ system
Electronic structure

Crystal structure

SrVO$_3$: $\angle V - O - V = 180^\circ$

↓

orthorhombic distortion

↓

CaVO$_3$: $\angle V - O - V \approx 162^\circ$

LDA density of states

SrVO$_3$

CaVO$_3$

No correlation effects/spectral transfer
LDA+DMFT results

$k$-integrated spectral function

constrained LDA: $U=5.55 \text{ eV}, J=1.0 \text{ eV}$

Osaka - Augsburg - Ekaterinburg collaboration:

How to measure?
Excursion: Spectroscopy

Photoemission Spectroscopy (PES)

Angular Resolved PES = ARPES

Measures occupied states of electronic spectral function
Ideal spectral function of a material
Occupied states
(ideal)
Occupied states (experiment)
Inverse Photoemission Spectroscopy (IPES)

Measures unoccupied states of electronic spectral function

Information also available by:

X-ray absorption spectroscopy (XAS)
Ideal spectral function of a material

IPES/XAS
IPES/XAS

Unoccupied states (ideal)

![XAS spectrum](image)
Unoccupied states (measured)
Comparison with experiment


- (i) bulk-sensitive high-resolution photoemission spectra (PES) $\rightarrow$ occupied states
- (ii) 1s x-ray absorption spectra (XAS) $\rightarrow$ unoccupied states
Surprising “kinks” in the quasiparticle dispersion $E_k$ at $\pm \omega_*$

- Purely electronic mechanism
- Generic for strong correlations

Kinks in high-resolution ARPES of Ni(110)
Perspective of DMFT approach

Explain and predict properties of complex correlated materials

Phase diagram of actinides
Perspective of DMFT approach

Explain and predict properties of complex correlated materials

Phase diagram of La$_{1-x}$Sr$_x$MnO$_3$

Hemberger et al. (2002)

1, 2, ... multi-electron transfer in metalloprotein complexes

→ Photosynthesis
**Perspective of DMFT approach**

Explain and predict properties of complex correlated materials

Phase diagram of \( \text{La}_{1-x}\text{Sr}_x\text{MnO}_3 \)

Hemberger *et al.* (2002)

1, 2, ..., multi-electron transfer in DNA

→ damage & repair
1. Quantum phase transitions

Driven by quantum fluctuations
1. Quantum phase transitions

- Non-Fermi liquid behavior
- Emergence of novel degrees of freedom
- New phases of matter

Driven by quantum fluctuations

Quantum critical point

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1. Quantum phase transitions

Driven by quantum fluctuations

- Non-Fermi liquid behavior
- Emergence of novel degrees of freedom
- New phases of matter

Custers et al. (2003)
2. Correlated electrons in non-equilibrium

Real-time evolution of correlation phenomena, e.g.,
time-resolved photoemission spectroscopy (PES)

Required: Theory of non-equilibrium beyond
linear response in correlated bulk materials

Perfetti et al. (2006)
2. Correlated electrons in non-equilibrium

Non-equilibrium DMFT

Schmidt, Monien (2002)
Freericks, Turkowski (2006)

Quench in Hubbard model from $U=0$ to $U>0$

Eckstein, Kollar, Werner (2009)

Momentum distribution ($U=3.3$)

Thermalization
3. Correlated cold atoms in optical lattices

Bosonic/fermionic atoms in optical lattices: Exp. realization of models

High degree of tunability: “quantum simulator”

Observation of Fermi surface (^{40}K atoms) Köhl, Esslinger (2006)
3. Correlated cold atoms in optical lattices

Hubbard model with ultracold atoms  Jaksch et al. (1998)

Angular momentum $L^{\text{tot}} = F \rightarrow N = 2F + 1$ hyperfine states

$\rightarrow$ SU(N) Hubbard models  Honerkamp, Hofstetter (2004)

$N = 3$, e.g. $^6$Li, $U < 0$: Color superconductivity, “baryon formation (QCD)”  Rapp et al. (2006)
Correlated many-particle systems: More fascinating than ever