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 Interacting Many-Particle Systems
Interacting many-particle systems

Elementary ("bare") particles + fundamental interactions

\[ \text{\# particles } \mathcal{N} \rightarrow \infty \]

effective ("quasi") particles + effective interactions
Non-interacting electrons

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

\[ \mathcal{N} \rightarrow \infty \]

Pauli exclusion principle of many fermions

Fermi-Dirac statistics

Ground state: Ferrari body/surface
Fermi gas: **Ground state**

- Fermi surface
- Fermi body
Fermi gas: **Excited state**

Switch on repulsive interaction

$k$-eigenstates: *infinite* life time

**Switch on repulsive interaction**
Fermi liquid

"Standard model of condensed matter physics"

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

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

(Quasi-) Particle = elementary excitation

Landau (1956/58)

Fermi surface \((k_F)\) \rightarrow

Fermi body

\[ k_x \]

\[ k_y \]

\[ k_z \]
Simple metals

"Heavy Fermions"

Potassium

\[ C/T = 2.08 + 2.57 T^2 \]

\[ m^* \approx m \]

Result of elementary excitations (quasiparticles)

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

Steglich et al. (1979)

\[ m^* \approx 1000 m \]

Stewart et al. (1983)

CeCu$_2$Si$_2$, UBe$_{13}$: very heavy quasiparticles
Interacting many-particle systems

Elementary ("bare") particles + fundamental interactions

\[ \downarrow \quad \text{\# particles } N \rightarrow \infty \]

effective ("quasi") particles + effective interactions

Vacuum

Coulomb potential

\[ \frac{Q}{r} \]
Interacting many-particle systems

Elementary ("bare") particles + fundamental interactions

\[
\downarrow \quad \# \text{ particles } N \to \infty
\]

effective ("quasi") particles + effective interactions

**Electron gas: Screening**

Simplest approximation: Thomas-Fermi

\[
Q \cdot e^{-r/\xi}
\]

Effective Yukawa potential
Interacting many-particle systems

Elementary ("bare") particles + fundamental interactions

\[ \downarrow \quad \text{\# particles } N \rightarrow \infty \]

effective ("quasi") particles + effective interactions

Electron gas: Screening
Better approximation: Lindhard

Friedel oscillations

\[ \frac{Q}{r^3} \cos(2k_F r) \]
Interacting many-particle systems

Elementary ("bare") particles + fundamental interactions

\[ \downarrow \quad \text{# particles } N \to \infty \]

effective ("quasi") particles + effective interactions

Electrons in real solids

"Strong effective interaction" of electrons in localized orbitals

Held (2004)
Interacting many-particle systems

\[ N \to \infty \]

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)
Interacting many-particle systems

# particles \( N \rightarrow \infty \)

Emergence

Examples:

- Superconductivity
- Magnetism
- Galaxy formation
- Traffic
- Weather
- Stock market
- Ants
- Human body
- Consciousness
Correlations
Correlation [lat.]: con + relatio ("with relation")

Grammar: either ... or

Correlations in mathematics, natural sciences:

$$\langle AB \rangle \neq \langle A \rangle \langle B \rangle$$

e.g., densities:

$$\langle \rho(r)\rho(r') \rangle \neq \langle \rho(r) \rangle \langle \rho(r') \rangle$$

Correlations:
Effects beyond factorization approximations (e.g., Hartree-Fock)
Temporal/spatial correlations in everyday life

But: External periodic potential + all states occupied
Temporal/spatial correlations in everyday life

But: External field
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

with

Technological applications:
- sensors, switches
- magnetic storage
- thermoelectrics
- functional materials, …
Electronic Correlations: Models
$H = -t \sum_{\langle i,j \rangle, \sigma} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$

Purely numerical approaches (d=2,3): hopeless

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

Static (Hartree-Fock-type) mean-field theories generally insufficient

Hubbard model

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

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

Hubbard model

Face-centered cubic lattice (d=3)

\[ Z=12 \]

Self-consistency problem

Dynamical single-site mean-field theory

Müller-Hartmann (1989); Brandt, Mielsch (1989); Janiš (1991); Janiš, DV (1992)
**Theory of correlated electrons**

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

Hubbard model

**Face-centered cubic lattice (d=3)**

Georges, Kotliar (1992); Jarrell (1992)

Self-consistent single-impurity Anderson model

Self-consistency problem

Strong simplifications

Metzner, DV (1989)

\( d, Z \to \infty \)

\( Z=12 \)
Dynamical mean-field theory (DMFT) of correlated electrons

Proper time resolved treatment of local electronic interactions

“Spectral transfer”

Experimentally detectable?
Correlated Electron: Materials
How to combine?

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

Held (2004)

How to combine?

time-averaged electron density

lattice potential

Held (2004)
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)
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

No correlation effects/spectral transfer
LDA+DMFT results

SrVO$_3$ / CaVO$_3$

k-integrated spectral function

![Graph showing SrVO$_3$ and CaVO$_3$ spectral functions](graph.png)

Constrained LDA: U=5.55 eV, J=1.0 eV

Osaka - Augsburg - Ekaterinburg collaboration:

Measure by spectroscopy
Comparison with experiment


Bulk sensitive photoemission spectroscopy → occupied states

X-ray absorption spectroscopy → unoccupied states

3-peak structure detected
\[ \omega_* = Z_{FL} D_{LDA} \quad \text{LDA bandwidth} \]
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)  
Hofmann et al.; PRL (2009)
State-of-the-art LDA+DMFT:
Electronic correlations & structural transformations

Electron correlations can induce structural transformations

Electronic correlations at the $\alpha$-$\gamma$ structural phase transition in paramagnetic iron

I. Leonov,¹ A. I. Poteryaev,² V. I. Anisimov,² and D. Vollhardt¹

arXiv:1008.4342
Phase diagram of actinides

Perspective of the LDA+DMFT approach

Explain and predict properties of complex correlated materials
Perspective of the LDA+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
Field induced quantum phase transition

- Driven by quantum fluctuations
  - Non-Fermi liquid behavior
  - Emergence of novel degrees of freedom
  - New phases of matter
Driven by quantum fluctuations

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


Si, Steglich (2010)
2. Correlated electrons in non-equilibrium

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

Required: Theory of non-equilibrium beyond linear response in correlated bulk materials
2. Correlated electrons in non-equilibrium

Non-equilibrium DMFT

Freericks, Turkowski (2006)

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

Eckstein, Kollar, Werner (2009)

Momentum distribution ($U=3.3$)

Eckstein, Kollar (2008)

Freericks, Krishnamurthy, Pruschke (2008)

Application, e.g.
- time resolved PES
- pump-probe experiments
3. Correlated cold atoms in optical lattices

Observation of Fermi surface (\(^{40}\)K atoms) Köhl, Esslinger (2006)

High degree of tunability: “quantum simulator”

Greiner et al. (2002)
3. Correlated cold atoms in optical lattices

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

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

$\rightarrow$ SU(N) Hubbard models  

$N=3$, e.g. $^6$Li, $U<0$: Color superconductivity, “baryon formation (QCD)”  
Rapp et al. (2006)

- trions
- Cooper pairs
Correlated many-particle systems: More fascinating than ever