Surprising Effects of Electronic Correlations in Solids

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Outline:

- Peculiarities of quantum many-particle systems
- Electronic correlations in solids
- Dynamical mean-field theory: Models vs. materials
- Other developments & perspectives
Example: *Magnetite* \((\text{Fe}_3\text{O}_4)\)

**Microscopic explanation of the physical properties?**

\(O(10^{23})\) interacting electrons + ions

→ quantum many-particle problem
Peculiarities of Interacting Many-Particle Systems
Interacting many-particle systems

Elementary ("bare") particles + fundamental interactions

↓

# particles $N \rightarrow \infty$

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

Spin = $\frac{1}{2} \hbar$ Fermion

$\Downarrow \quad N \rightarrow \infty$, Pauli exclusion principle

Fermi-Dirac statistics

$\Downarrow$

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

Fermi surface $\rightarrow$

$$E_F = \frac{\hbar^2}{2m} k_F^2$$

Fermi sphere

$$\frac{E_0}{N} = \frac{3}{5} E_F \implies \text{Fermi pressure } P_{\text{Fermi}} = -\frac{\partial E_0}{\partial V} = \frac{2}{5} \frac{N}{V} E_F > 0$$

Incompressibility of ordinary matter due to Pauli principle + uncertainty relation
Fermi gas: **Excited state**

Switch on repulsive interaction

$k$-eigenstates: *infinite* life time
Fermi liquid

Well-defined \( k \)-states ("quasiparticles") with

- finite life time
- effective mass \( m^* \)
- effective interaction

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

(Quasi-) Paticle = elementary excitation

Landau (1956/58)

Fermi sphere

Fermi surface

"Standard model of condensed matter physics"
Simple metals

Potassium

\[ m^* \approx m \]

 POTASSIUM

\[
\lim_{T \to 0} \frac{c_V}{T} = \gamma \propto \frac{m^*}{m}
\]

Result of elementary excitations (quasiparticles)

"Heavy Fermions"

Steglich et al. (1979)

\[ m^* \approx 1000 \, m \]

Stewart et al. (1983)

\[ \text{CeCu}_2\text{Si}_2, \, \text{UBe}_{13}: \]

very heavy quasiparticles (Kondo impurity physics)
Interacting many-particle systems

Elementary ("bare") particles + fundamental interactions

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

effective ("quasi") particles + effective interactions

Vacuum

\[
Q \quad r \quad O \quad r
\]

Coulomb potential
Interacting many-particle systems

Elementary ("bare") particles + fundamental interactions

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

effective ("quasi") particles + effective interactions

Electron gas: Screening
Simplest approximation: Thomas-Fermi

Effective Yukawa potential
Interacting many-particle systems

Elementary ("bare") particles + fundamental interactions

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

effective ("quasi") particles + effective interactions

Electron gas: Screening
Better approximation: Lindhard

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

Friedel oscillations
Electrons in real solids

Elementary ("bare") particles + fundamental interactions

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

effective ("quasi") particles + effective interactions

"Strong effective interaction" of electrons in localized orbitals
... but “dirt physics” can be fundamental and universal

Magnetic impurity in a host of non-interacting (mobile) electrons

T > T_K (high energies)
Asymptotically free local moment

T < T_K (low energies)
Screening of moment (confinement)

“Kondo effect”

\[
T_K \sim E_F e^{-1/|J(\Lambda)| N(E_F)}
\]

Prototypical interaction problem with “running coupling constant” \( J(\Lambda) \)
\( \rightarrow \) QED, QCD

- “Die Festkörperphysik ist eine Schmutzphysik” (Pauli)
- “One shouldn’t wallow in dirt” (Pauli to Peierls, 1929)
Entirely new phenomena, e.g., phase transitions

Unpredicted behavior “emerges”

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'.
Eddington (1882-1944)

“More is different” Anderson (1972)
Entirely new phenomena, e.g., phase transitions

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

Unpredicted behavior “emerges”

Examples:
- Superconductivity
- Magnetism
- Metal-insulator transition
- Traffic
- Weather
- Stock market
Interacting many-particle systems

$\downarrow \quad \# \text{ particles } N \rightarrow \infty$

Entirely new phenomena, e.g., phase transitions

\[ \text{Fe}_3\text{O}_4 \]

Metal-insulator transition

Strong effective repulsion of “electrons” (quasiparticles!): Correlation effect
Correlations
Correlation [lat.]: con + relatio ("with relation")

Correlations in mathematics, natural sciences:

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

e.g., densities:

\[ \langle n(\mathbf{r})n(\mathbf{r}') \rangle \neq \langle n(\mathbf{r}) \rangle \langle n(\mathbf{r}') \rangle = n^2 \]

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

Correlations?
Temporal/spatial correlations in everyday life

But: External periodic potential → long-range order enforced → no genuine correlations
Temporal/spatial correlations in everyday life

Time/space average (Hartree-Fock approximation) inappropriate
Electronic Correlations in Solids
Narrow d,f-orbitals/bands

Partial filled d-orbitals

Partial filled f-orbitals
Correlated electron materials have unusual properties

- huge resistivity changes
- gigantic volume anomalies
- colossal magnetoresistance
- high-$T_c$ superconductivity
- metallic behavior at interfaces of insulators

With potential for technological applications:

- sensors, switches
- spintronics
- thermoelectrics
- high-$T_c$ superconductor devices
- functional materials: oxide heterostructures ...

How to study correlated systems theoretically?
material

⇒ "realistic" model

⇒ maximal reduction: Hubbard model
Theoretical challenge of many-fermion problems:
Construct reliable, comprehensive non-perturbative approximation schemes

Hubbard model

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

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

\[ \langle n_{i\uparrow} n_{i\downarrow} \rangle \neq \langle n_{i\uparrow} \rangle \langle n_{i\downarrow} \rangle \]

Static (Hartree-Fock) mean-field theories generally insufficient
Non-perturbative approximation schemes for real materials

**DFT/LDA**

+ material specific: “ab initio”
+ fast code packages
- fails for strong correlations

**Model Hamiltonians**

- input parameters unknown
- computationally expensive
+ systematic many-body approach

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**How to combine?**

- time-averaged electron density
- lattice potential

Held (2004)
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-consistent single-impurity Anderson model

Georges, Kotliar (1992)
(i) Effective single-impurity problem: Local propagator

\[
G = -\frac{1}{Z} \int D[\psi, \psi^*] \psi \psi^* e^{\psi^* [G^{-1} + \Sigma]} \psi - U \psi^* \psi \psi^* \psi
\]

single-site ("impurity") action \(A\)

(ii) Lattice Green function

\[
G(\omega) = \int d\varepsilon \frac{N^0(\varepsilon)}{\omega - \Sigma(\omega) - \varepsilon} = G^0(\omega - \Sigma(\omega)) \\
\rightarrow \text{free electrons in a dynamic potential } \Sigma(\omega)
\]

Solve with an „impurity solver“, e.g., QMC, NRG, ED,…
Dynamical mean-field theory (DMFT) of correlated electrons

Exact time resolved treatment of local electronic interactions

Landau quasiparticles, not “electrons“
Dynamical mean-field theory (DMFT) of correlated electrons

Metzner, DV (1989)
Georges, Kotliar (1992)

Kotliar, DV (2004)

Exact time resolved treatment of local electronic interactions

Definition of Correlations (II):
Transfer of spectral weight

Experimentally detectable!
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 et al. (1997)
Lichtenstein, Katsnelson (1998)
Held et al. (2003)
Kotliar et al. (2006)
Computational scheme for correlated electron materials:

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

+ 

Local electronic correlations
(Many-body theory: DMFT)

= 

X + DMFT

X = LDA, GGA; GW, ...
1st Application of LDA+DMFT

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

Crystal structure

\( \text{SrVO}_3: \angle V - O - V = 180^\circ \)

\[ \angle V - O - V \approx 162^\circ \]

No correlation effects/spectral transfer
LDA+DMFT results

Spectral function

SrVO$_3$ / CaVO$_3$

Measure by spectroscopy

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

Comparison with experiment

Bulk sensitive photoemission spectroscopy → occupied states

X-ray absorption spectroscopy → unoccupied states

Fe

2\textsuperscript{nd} Application of LDA+DMFT

- Most abundant element by mass on Earth
- Ferromagnetism: Longest known quantum many-body phenomenon
- Still most widely used metal in modern day industry ("iron age")
Narrow d, f-orbitals/bands → electronic correlations important

Fe: Electronic configuration [Ar] 3d⁶4s²
Exceptional:

- Abundance of allotropes: $\alpha$, $\gamma$, $\delta$, $\varepsilon$, ... phases
- bcc-phase stable for P,T $\rightarrow 0$
- Very high Curie temperature ($T_C = 1043$ K)
Mikhaylushkin, Simak, Dubrovinsky, Dubrovinskaia, Johansson, Abrikosov (2007)
Until recently:
LDA+DMFT investigations of correlated materials for given lattice structure

- How do electrons + ions influence each other?
- Which lattice structure is stabilized?
Investigation of the structural stability of Fe

Collaborators:  Ivan Leonov (Augsburg)
               Vladimir Anisimov (Ekaterinburg)
               Alexander Poteryaev (Ekaterinburg)
DFT(GGA): finds paramagnetic $\text{bcc}$ phase to be unstable

- What stabilizes paramagnetic ferrite?
- What causes the $\text{bcc}$-$\text{fcc}$ structural phase transition?
LDA+DMFT: Electronic correlations responsible for $T_{\text{struct}} > T_C$

Leonov, Poteryaev, Anisimov, DV (2011)
Lattice dynamics of paramagnetic \textit{bcc} iron

Non-magnetic GGA phonon dispersion

Dynamically unstable + elastically unstable ($C_{11}, C' < 0$)

Experiment:
Neuhaus, Petry, Krimmel (1997)
Lattice dynamics of paramagnetic \textit{bcc} iron

- phonon frequencies calculated with frozen-phonon method
- harmonic approximation

GGA+DMFT phonon dispersion at 1.2 $T_C$

Calculated:
- equilibrium lattice constant $a \sim 2.883$ Å ($a_{\text{exp}} \sim 2.897$ Å)
- Debye temperature $\Theta \sim 458$ K

Theory:
Leonov, Poteryaev, Anisimov, DV (2012)

Experiment:
Neuhaus, Petry, Krimmel (1997)
Other Developments & Perspectives
Correlated electrons in non-equilibrium

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

Required: Theory of non-equilibrium in correlated bulk materials

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

Non-equilibrium DMFT

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

Momentum distribution ($U=3.3$)

Extension, e.g.
- time resolved PES
- pump-probe experiments

Eckstein, Kollar (2008)
Eckstein, Kollár (2008)
Freericks, Krishnamurthy, Pruschke (2008)
Correlated cold atoms in optical lattices

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

High degree of tunability: “quantum simulator” (Feynman, 1982)

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

Hubbard model with ultracold atoms
Jaksch, Bruder, Cirac, Gardiner, Zoller (1998)

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

$\rightarrow$ SU$(N)$ Hubbard models

$N=3$, e.g. $^6\text{Li}$, $U<0$: Color superconductivity, “baryon formation (QCD)”
Correlated cold atoms in optical lattices

Hubbard model with ultracold atoms

Jaksch, Bruder, Cirac, Gardiner, Zoller (1998)

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

$\rightarrow$ SU($N$) Hubbard models


How to implement local gauge invariance & relativistic structure?

Quantum simulations of lattice gauge theories:
Local gauge invariance from angular momentum conservation in atomic scattering processes

Zohar, Cirac, Reznik (2013)
Correlated many-particle systems: More fascinating than ever