Surprising Effects of the Interaction between Electrons in Matter

Dieter Vollhardt

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Outline:

1. Peculiarities of many-particle systems
2. Correlations
3. Electronic correlations in solids
4. Dynamical Mean-Field Theory: Models vs. materials
5. New Developments & Perspectives

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1. Peculiarities of Many-Particle Systems
Interacting many-particle systems

Elementary ("bare") particles + interactions

\[ N \to \infty \]

effective ("quasi") particles + effective interactions

Vacuum

Coulomb potential

\[ \frac{e^2}{r} \]
Interacting many-particle systems

Elementary ("bare") particles + 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 + interactions

\[ N \rightarrow \infty \]

Effective ("quasi") particles + effective interactions

Electron gas: Screening
Better approximation: Lindhard

Friedel oscillations

\[ \frac{e^2}{r^3} \cos(2k_F r) \]
Electrons in solids

Interacting many-particle systems

Elementary ("bare") particles + interactions

\[ N \rightarrow \infty \]

effective ("quasi") particles + effective interactions

"Strong interaction" of electrons in localized orbitals

\( \uparrow \)

Coulomb interaction \( \Rightarrow \) correlations
Quasiparticles
Electrons

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

\Downarrow

\Downarrow

\text{Fermi-Dirac statistics}

\Downarrow

\text{Pauli exclusion principle of many fermions}

\text{Fermi body/surface}
Fermi gas: **Ground state**

Fermi surface →

Fermi sea

$\mathbf{k}_x$, $\mathbf{k}_y$, $\mathbf{k}_z$
Fermi gas: **Excited states** ($T>0$)

Switch on interaction adiabatically ($d=3$)

Exact $k$-states ("particles"): *infinite* life time

**Switch on interaction adiabatically** ($d=3$)
Landau Fermi liquid

1-1 correspondence between $k$-states

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

Landau (1956/58)
Simple metals

Consequence of elementary excitations (quasiparticles)

\[ \lim_{T \to 0} \frac{C_V}{T} \approx \gamma_0 \Rightarrow m^* \approx m \]

"Heavy Fermions"

Steglich et al. (1979)

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

Stewart et al. (1983)

CeCu\textsubscript{2}Si\textsubscript{2}, UBe\textsubscript{13}:

strongly interacting electrons

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

$N \rightarrow \infty$

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

$N \to \infty$

Emergence

Examples:

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

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2. Correlations
Correlation [lat.]: \textit{con + relatio} ("with relation")

Grammar: \textit{either ... or}

Mathematics, natural sciences:

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

e.g., densities:

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

Time/space average insufficient
Correlations vs. long-range order

_Sempe, THE NEW YORKER_
3. Electronic Correlations in Solids
Partially filled d-orbitals

Partially filled f-orbitals

Narrow d, f-orbitals/bands → strong electronic correlations
### Electronic Bands in Solids

#### Insulator
- **Property**: Atomic levels
- **Representation**: Localized electrons $n_{i\sigma}$
- **Example**: Solid Ne NaCl

#### Correlated metal
- **Property**: Narrow bands
- **Representation**: $n_{i\sigma} \leftrightarrow n_{k\sigma}$
- **Example**: Transition + rare earth metals/oxides (Ni, V$_2$O$_3$, Ce)

#### Simple metal
- **Property**: Broad bands
- **Representation**: Extended waves $n_{k\sigma}$
- **Example**: Na, Al

#### Average time spent on atom
$$\tau \sim \frac{\hbar}{W}$$

#### Narrow band → small $W$: Strong electronic correlations

<table>
<thead>
<tr>
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<th>Energy levels</th>
<th>Representation</th>
<th>Example</th>
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Correlated electron materials

Fascinating topics for fundamental research

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

with

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

Local Hubbard physics:
Static (Hartree-Fock) mean-field theories generally insufficient

Correlation phenomena:
Metal-insulator transition, ...

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

Local Hubbard physics:
\[ \langle n_{i\uparrow} n_{i\downarrow} \rangle \neq \langle n_{i\uparrow} \rangle \langle n_{i\downarrow} \rangle \]

Static (Hartree-Fock) mean-field theories generally insufficient
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Main theoretical challenge: Construct reliable, comprehensive approximation schemes.

Local Hubbard physics:

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

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

Static (Hartree-Fock) mean-field theories generally insufficient.
4. Dynamical Mean-Field Theory (DMFT) of Correlated Electrons
Theory of strongly correlated electrons

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

Hubbard model

Hypercubic lattices: Coordination number \( Z=2d \)

Dimension \( d=1 \)

\( Z=2 \)
Theory of strongly correlated electrons

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

Hubbard model

Hypercubic lattices: Coordination number \( Z = 2d \)

Dimension \( d = 2 \)

\[ Z = 4 \]
Theory of strongly correlated electrons

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

Hubbard model

Hypercubic lattices: Coordination number \( Z = 2d \)

Dimension \( d = 3 \)

\( Z = 6 \)
Theorem of strongly correlated electrons

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

Hubbard model

Body-centered cubic lattice

Dimension \( d = 3 \)

\( Z = 8 \)
Theory of strongly correlated electrons

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

Hubbard model

Face-centered cubic lattice

Dimension d=3

Metzner, DV (1989)


Georges and Kotliar (1992)

“Dynamical mean-field theory“
Dynamical mean-field theory of correlated electrons

Proper time resolved treatment of local electronic interactions:

Physics Today
Kotliar, DV (2004)

Experimentally measurable?
Correlated Electron: Materials
DFT/LDA

+ material specific: "ab initio"
- fails for strong correlations
+ fast code packages
How to combine?

**DFT/LDA**
- Material specific: “ab initio”
- Fails for strong correlations
- Fast code packages

**Model Hamiltonians**
- Input parameters unknown
- Systematic many-body approach
- Computationally expensive

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How to combine?

- Time-averaged electron density
- Lattice potential

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Coulomb interaction

Correlations

Held (2004)
Computational scheme for correlated electron materials:

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

+ 

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

→ **LDA+DMFT**

References:

- Anisimov *et al.* (1997)
- Lichtenstein, Katsnelson (1998)
- Nekrasov *et al.* (2000)

- Kotliar *et al.* (RMP, 2006)
Application of LDA+DMFT:
(Sr,Ca)VO$_3$
Electronic structure

Crystal structure

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

$\downarrow$

orthorhombic distortion

$\downarrow$

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

LDA density of states

SrVO$_3$

- $V$-3d$_{t_{2g}}$
- $V$-3d$_{e_g}$

CaVO$_3$

- $V$-3d$_{t_{2g}}$
- $V$-3d$_{e_g}$

No correlation effects/spectral transfer
LDA+DMFT results

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


How to measure?
Excursion: Spectroscopy

1. Photoemission Spectroscopy (PES)

Angular Resolved PES = ARPES

Measures occupied states of electronic spectral function
Ideal spectral function of a material
Ideal spectral function of a material
Occupied states
(ideal)
Occupied states (experiment)
2. **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
Unoccupied states (ideal)
Unoccupied states
(measured)

- (i) bulk-sensitive high-resolution photoemission spectra (PES)
- (ii) 1s x-ray absorption spectra (XAS) → unoccupied states
SrVO$_3$ and CaVO$_3$


“Kinks” in the quasiparticle dispersion $E_k$ at $\pm \omega_*$

$\omega_* = Z_{FL} D_{LDA}$

LDA bandwidth

Kinks in high-resolution ARPES of Ni(110)

5. New Developments & Perspectives
(i) Complex correlated electron materials

Explanation & prediction of properties of complex materials

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

Hemberger *et al.* (2002)

Kagome layer in ZnCu$_3$(OH)$_6$Cl$_2$
(herbertsmithite): Spin liquid behavior

1, 2, ... multi-electron transfer in metalloprotein complexes → Photosynthesis
(i) Complex correlated electron materials

Explanation & prediction of properties of complex materials

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

Hemberger et al. (2002)

Kagome layer in $\text{ZnCu}_3(\text{OH})_6\text{Cl}_2$
(herbertsmithite):
Spin liquid behavior

1, 2, ... multi-electron transfer in DNA
→ damage & repair
(ii) Quantum phase transitions

Driven by quantum fluctuations

- Non-Fermi liquid behavior
- Emergence of novel degrees of freedom
- New phases of matter
(ii) Quantum phase transitions

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

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(Augsburg-Dresden-Göttingen-Karlsruhe-Köln-München, 2007)
(ii) Quantum phase transitions

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

Driven by quantum fluctuations

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

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

Pump-probe experiment

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

Perfetti et al. (2006)
(iv) Correlated fermionic/bosonic atoms in optical lattices

Modugno et al. (2003)

Köhl, Esslinger (2006)

Bosonic/fermionic atoms in optical lattices

Observation of Fermi surface ($^{40}$K atoms)

High degree of tunability: “Many-body tool box”
(iv) Correlated fermionic/bosonic 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  

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