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
- Other Developments & Perspectives
Peculiarities of Many-Particle Systems
Interacting many-particle systems

Elementary ("bare") particles + fundamental interactions

\[ N \rightarrow \infty \]

effective ("quasi") particles + effective interactions

Vacuum

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

Coulomb potential
Interacting many-particle systems

Elementary ("bare") particles + fundamental interactions

\[ N \rightarrow \infty \]

effective ("quasi") particles + effective interactions

Electron gas: Screening
Simplest approximation: Thomas-Fermi

Effective Yukawa potential

\[ \frac{Q}{r} e^{-r/\xi} \]
Interacting many-particle systems

Elementary ("bare") particles + fundamental interactions

$N \rightarrow \infty$

effective ("quasi") particles + effective interactions

Electron gas: Screening
Better approximation: Lindhard

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

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

Held (2004)
Quasiparticles
Electrons

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

\[ \Downarrow \]

Fermi-Dirac statistics

\[ \Downarrow \quad \text{Pauli exclusion principle of many fermions} \]

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

![Diagram of Fermi gas with Fermi surface and Fermi sea](image)

- **Fermi surface**
- **Fermi sea**

$k_x$, $k_y$, $k_z$
Fermi gas: **Excited states** (T>0)

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

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

Landau (1956/58)

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

(Quasi-) Particle

= elementary excitation

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

Fermi surface

\((\text{Quasi-})\) Hole

\(\text{Fermi sea}\)
Simple metals

Result 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)

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)
Emergence

Examples:

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

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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:

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

Correlations
Temporal/spatial correlations in everyday life
Electronic Correlations in Solids
Partial filled d-orbitals

Partial filled f-orbitals

Narrow d,f-orbitals/bands $\rightarrow$ 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
$H = -t \sum_{\langle i,j \rangle, \sigma} c_i^{\dagger} c_j^{\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$

Hubbard model

Gutzwiller, 1963
Hubbard, 1963
Kanamori, 1963
Hubbard model

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

Gutzwiller, 1963
Hubbard, 1963
Kanamori, 1963
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: hopeless

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

Gutzwiller, 1963
Hubbard, 1963
Kanamori, 1963

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

Face-centered cubic lattice

Dimension \( d = 3 \)

\( Z = 12 \)

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

Müller-Hartmann (1989); Brandt and Mielsch (1989); Janis (1991); Georges and Kotliar (1992); Jarrell (1992)
Proper time resolved treatment of local electronic interactions:

Dynamical mean-field theory (DMFT) of correlated electrons

“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)
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$_3$
Electronic structure

Crystal structure

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

↓

orthorhombic distortion

↓

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

No correlation effects/spectral transfer
LDA+DMFT results

$k$-integrated spectral function

SrVO$_3$ and CaVO$_3$

constrained LDA:
$U=5.55$ eV, $J=1.0$ 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
Unoccupied states (ideal)
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 $\pm \omega_*$

Kinks in high-resolution ARPES of Ni(110)

**Phase diagram of actinides**

**Perspective of DMFT approach**

Explain and predict properties of complex correlated materials
**Perspective of DMFT approach**

Explain and predict properties of complex correlated materials

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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 metalloprotein complexes

$\rightarrow$ 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)

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
Other Developments
1. Quantum phase transitions

- Non-Fermi liquid
- Quantum critical

Driven by quantum fluctuations
1. Quantum phase transitions

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

Driven by quantum fluctuations

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1. Quantum phase transitions

Custers et al. (2003)

Fermi-liquid instabilities at magnetic quantum phase transitions

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

Pump-probe experiments:

1\textsuperscript{st} light pulse: Pumps into non-equilibrium state
2\textsuperscript{nd} light pulse: Probes to study relaxation

Pulse duration $\delta$ $\leftrightarrow$
Energy resolution $\Delta E \approx \hbar / \delta$

\begin{align*}
\delta &= 0.33 \\
\text{Decent time and energy resolution}
\end{align*}

Mott insulator (FK model, $U=10$)
photo-excited into metallic state ($U=1$):

- Initial metallic state
- Decent time and energy resolution

Oscillation period $\frac{2\pi \hbar}{U}$

Eckstein, Kollar (2008)
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)

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

Hubbard model with ultracold atoms

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

$\to$ SU(N) Hubbard models

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

Jaksch et al. (1998)


Rapp et al. (2006)
Correlated many-particle systems:

More fascinating than ever