PREHISTORY OF THE HUBBARD MODEL

Memories of John Hubbard
Motivation for the model
Its impact

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JOHN HUBBARD (1931-1980) biography

1949-52 Undergraduate in Mathematics Department, Imperial College London
1952-55 Postgraduate in Mathematics Department, Imperial College London (PhD supervisors Harry Jones and Stanley Raimes)
1955-76 AERE Harwell
1976-80 IBM Research Laboratory, San Jose
Hubbard’s favourite machine (1952-55)
Marchant Figurematic
Electron correlations in narrow energy bands

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Motivation: Magnetism in ferromagnetic transition metals. Disordered local moments above $T_c$.

Spin waves

These phenomena most easily explained by a localized Heisenberg model and some (Van Vleck, Stoner, Wohlfarth) doubted the existence of spin waves in metals. Their direct observation in iron by neutron scattering at Harwell (Lowde 1956) convinced many (but not all?).
Hubbard was impressed by the description in the indicated papers of a spin wave as correlation (a bound state) between a minority spin electron and a majority spin hole. He sought a more general description of electron correlation in narrow energy bands. He only achieved a theory of disordered moments above $T_c$ in his last papers.

No mention of Mott’s papers on the metal-insulator transition; this came a year later in Hubbard III after discussions with Mott.
THE HUBBARD MODEL:

\[ H = \sum_{i,j} \sum_{\sigma} T_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \frac{1}{2} I \sum_{i,\sigma} n_{i\sigma} n_{i,-\sigma} \]

THE HUBBARD U!

The model combines a tight-binding s-band with an onsite Coulomb interaction and has a prehistory, notably in Slater’s (1937) work on spin waves in a ferromagnetic insulator where the ground state comprises a full majority spin band. Slater also included a nearest neighbour direct exchange term. The problem of one reversed spin is a soluble 2-body problem:
Ferromagnetic insulator

One reversed spin

Stoner excitations

Spin waves

Energy of lowest state:

\[ E_0 + A \sum_\mathbf{R} (1 - \cos \mathbf{K} \cdot \mathbf{R}) \]

Where

\[ A = I_0 - 2W_R^2/I_1 \]

(31)

Direct exchange

Anderson superexchange: \(-2t^2/U\)

Simplest Green’s function decoupling with correct $U=0$ and $t=0$ limits.

NEW RESULTS:

HUBBARD SPLITTING OF BAND. GAP APPEARS FOR ALL $U > 0$.
(Improved in Hubbard III with discussion of Mott transition)

CONDITION FOR FERROMAGNETISM $U_{\text{eff}} P(\mu) > 1$
with $U_{\text{eff}} \sim$ bandwidth for large $U$
(cf Kanamori 1963, Callaway and Edwards 1964)
Alloy analogy $U n_{i\uparrow} <n_{i\downarrow}>$, configurational average, CPA. One-electron CPA for alloys didn’t exist in 1964 so Hubbard invented a many-body CPA using Green’s function equations of motion. Basic approximations $[H, n_{i\downarrow}] = 0$ and a self-consistency argument. Mott transition at critical bandwidth/ $U$ ratio.

$${\mathcal H} = \sum_{ij\sigma} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$
Hubbard’s many-body CPA (local approximation, self-energy a function of energy only) paved the way for dynamical mean-field theory (DMFT) which came nearly 30 years later. (Janis 1991, Georges and Kotliar 1992, Janis and Vollhardt 1992). We needed extensions of the Hubbard III method to use CPA for the double exchange (DE) and Holstein-DE models for manganites (review in Adv. Phys. 51 1259 (2002). But Hubbard’s (1964) metallic state was not a Fermi liquid owing to the alloy analogy (no quasiparticles of infinite lifetime at the Fermi surface and hence no Migdal discontinuity). How to introduce ↓-spin dynamics correctly? Not possible by Hubbard’s EOM decoupling method and my personal path to DMFT (after earlier work with John Hertz) was an exact diagrammatic treatment of the self-energy within the local approximation (J. Phys.: Condensed Matter 5 161 (1993). Diagrams the same for all models with the Hubbard U interaction e.g. Hubbard model, Anderson impurity model, Anderson lattice.
We can show that the self-energy $\Sigma$ for a given model is given by

$$\Sigma = S[G/(1+G\Sigma)]$$

where $S$ is a functional defined by a certain set of diagrams and $G$ is the full local Green’s function. If we assume that the functional $S$ is model-independent (true for dimension $d=\infty$) we can determine it by reference to the impurity model for which

$$G/(1+G\Sigma) = G^0$$

where $G^0$ is the Green’s function for the non-interacting system. Thus

$$\Sigma_{\text{imp}} = S[G_{\text{imp}}^0]$$

which determines the functional $S$ if we can calculate the self-energy for the impurity model with arbitrary unperturbed propagator or, equivalently, arbitrary hybridization function $\Delta(E)$. For the Hubbard model $G=G^0(E-\Sigma)$ and this procedure can describe the Mott transition with a proper Fermi liquid in the metallic state.

**Hubbard III pointed in the right direction**

*(in the alloy analogy approximation $S$ is a universal function)*

$$S^{\text{AA}}[G] = U <n_\downarrow>/[1-(1-n_\downarrow)UG]$$
1979-1980 Hubbard returns to the main motivation for Hubbard I:

Magnetism in transition metals,
Disordered local moments at finite temperature.

Ingredients of the theory: Hubbard Hamiltonian, functional integral method (Hubbard-Stratonovitch PRL 3 77 (1959)) introducing time-dependent local exchange fields, static approximation and CPA averaging (cf. alloy analogy), U replaced by effective parameter to give correct ground state moment.

Hasegawa did similar theory at the same time. Physical picture:
In functional integral method the Hubbard interaction can be written in four ways which give different answers after the static approximation. Hubbard wanted to use (d) (rotationally invariant and correct HF at T=0) but some correct results for this only appear in a Taniguchi symposium proceedings, not in four other papers (3 PRB, 1 JAP)!

\[ \sum_{i \uparrow \downarrow} n_{i \uparrow} n_{i \downarrow} = \frac{1}{2} \sum_{i} n_{i \uparrow} - 2 \sum_{i} (S_{i}^{z})^2 \]  
\[ = \frac{1}{4} \sum_{i} n_{i \uparrow}^2 - \sum_{i} (\frac{e_{i}}{n_{i \downarrow}^2})^2 \]  
\[ = \frac{1}{4} \sum_{i} n_{i \uparrow}^2 - \frac{1}{3} \sum_{i} S_{i}^2 \]  
\[ = \frac{1}{4} \sum_{i} n_{i \uparrow}^2 - \sum_{i} (\frac{e_{i} \cdot S_{i}}{n_{i \downarrow}})^2 \]  

arbitrary unit vector, direction averaged over at end of calculation
Electron Correlation and Magnetism in Narrow-Band Systems

Proceedings of the Third Taniguchi International Symposium, Mount Fuji, Japan, November 1-5, 1980

Editor: T. Moriya
Springer-Verlag Berlin Heidelberg New York 1981

Calculation of the Magnetic Properties of Iron and Nickel by the Functional Integral Method

John Hubbard*
IBM Research Laboratory, San Jose, CA 95193, USA

*John Hubbard died on November 27, 1980, and this paper has been prepared from his notes by D.M. Edwards
Results presented by John Hubbard at the Taniguchi Symposium (Nov. 1-5, 1980)

Values of $T_c$ obtained are given in the following table:

<table>
<thead>
<tr>
<th>Method</th>
<th>Metal</th>
<th>Calculated (K)</th>
<th>Observed (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(c)</td>
<td>Fe</td>
<td>1840</td>
<td>1044</td>
</tr>
<tr>
<td>(c)</td>
<td>Ni</td>
<td>1200</td>
<td>630</td>
</tr>
<tr>
<td>(d)</td>
<td>Ni</td>
<td>578</td>
<td>630</td>
</tr>
</tbody>
</table>
Fig. 3 The root-mean-square atomic spin magnitude $S(T)$ calculated for nickel by methods (c) and (d), as a function of temperature; $S(0)$ equals the ground state spin.

Fig. 4 The distribution functions $P(S)$ for the atomic spin lengths calculated for iron and nickel in the paramagnetic region; $S(0)$ is the ground state atomic spin and curves (c) for nickel and iron show $P(S)S(0)$ rather than $P(S)$. 
Participants in the Taniguchi International Symposium, November 1 - 5, 1980
(photographed with Mt. Fuji in the background)

Seated (left to right)
T. Moriya  A. Yanase  J. A. Hertz  J. Hubbard  R. Kubo  Mrs. Prange
D. M. Edwards  K. Yosida  T. Kasuya  K. Yamada

Standing (left to right)
O. Nakanishi  K. Ueda  K. Kubo  J. Igarashi  E. Müller-Hartmann
F. D. M. Haldane  C. P. Enz  J. Kanamori  R. E. Prange  H. Hasegawa
Y. Takahashi  K. Usami
CONCLUDING REMARKS

The Hubbard model had a prehistory e.g. Slater (1937) but Hubbard I (1963) launched the general subject of “strongly correlated electron systems”.

A non-perturbative treatment of the one-particle Green’s function led to “Hubbard splitting” and provided the first formalism for discussing the Mott transition.

Hubbard III (1964) introduced many-body CPA leading towards DMFT and a better theory of the Mott transition.

Hubbard (1978-80) used his model, combined with Hubbard-Stratonovich and CPA, to give the first satisfactory theory of transition metal magnetism at finite temperature.

Sriram Shastry will show us later how John Hubbard’s unique legacy lives on.