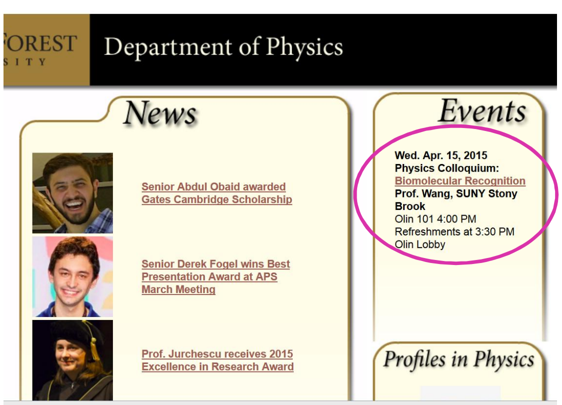
PHY 752 Solid State Physics
11-11:50 AM MWF Olin 107

Plan for Lecture 32:

- The Hubbard model
  - Motivation for the model
  - Solution for a 2 site system
  - Hartree-Fock approximation
  - Comparison with exact solutions

20	Mon: 03/16/2015		Review Mid-term exam	#19	03/18/2015
21	Wed: 03/18/2015	Chap. 16	Electron Transport	#20	03/20/2015
22	Fri: 03/20/2015	Chap. 16	Electron Transport	#21	03/23/2015
23	Mon: 03/23/2015	Chap. 17	Electron Transport	#22	03/25/2015
24	Wed: 03/25/2015	Chap. 17 & 18	Electron Transport		
25	Fri: 03/27/2015	Chap. 18	Microscopic picture of transport	#23	03/30/2015
26	Mon: 03/30/2015	Chap. 19	Semiconductor devices	#24	04/01/2015
27	Wed: 04/01/2015	Chap. 20	Models of dielectric functions	#25	04/06/2015
	Fri: 04/03/2015	Good Friday	No class		
28	Mon: 04/06/2015	Chap. 21	Optical properties of solids	#26	04/08/2015
29	Wed: 04/08/2015	Chap. 22	Modern theory of polorization	#27	04/10/2015
30	Fri: 04/10/2015		Surface properties of solids	#28	04/13/2015
31	Mon: 04/13/2015		X-ray and neutron diffraction in solids	#29	04/15/2015
32	Wed: 04/15/2015	Chap. 26	The Hubbard model	#30	04/17/2015
33	Fri: 04/17/2015				04/20/2015
34	Mon: 04/20/2015				
35	Wed: 04/22/2015				
36	Fri: 04/24/2015				
	Mon: 04/27/2015		Presentations I		
	Wed: 04/29/2015		Presentations II		
	Fri: 05/01/2015		Presentations III & Take home exam		



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Electron Correlations in Narrow Energy Bands
Author(s): J. Hubbard
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Electron correlations in narrow energy bands

By J. Hubbard
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(*Communicated by B. H. Flowers, F.R.S.—Received* 23 *April* 1963)

It is pointed out that one of the main effects of correlation phenomena in *d*- and *f*-bands is to give rise to behaviour characteristic of the atomic or Heitler–London model. To investigate this situation a simple, approximate model for the interaction of electrons in narrow energy bands is introduced. The results of applying the Hartree–Fock approximation to this model are examined. Using a Green function technique an approximate solution of the correlation problem for this model is obtained. This solution has the property of reducing to the exact atomic solution in the appropriate limit and to the ordinary uncorrelated band picture in the opposite limit. The condition for ferromagnetism of this solution is discussed. To clarify the physical meaning of the solution a two-electron example is examined.

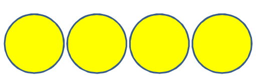
The Hubbard Hamiltonian:

$$\hat{\mathcal{H}} = \sum_{\substack{\langle ll' \rangle \\ \sigma}} -t \left[\hat{c}^\dagger_{l\sigma} \hat{c}_{l'\sigma} + \hat{c}^\dagger_{l'\sigma} \hat{c}_{l\sigma} \right] + U \sum_{l} \hat{c}^\dagger_{l\uparrow} \hat{c}_{l\uparrow} \hat{c}^\dagger_{l\downarrow} \hat{c}_{l\downarrow},$$

single particle contribution

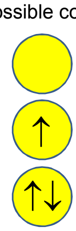
two particle contribution

$$\{c_{l\sigma}, c_{l'\sigma'}\} = 0$$
$$\{c^\dagger{}_{l\sigma}, c^\dagger{}_{l'\sigma'}\} = 0$$
$$\{c_{l\sigma}, c^\dagger{}_{l'\sigma'}\} = \delta_{ll'}\delta_{\sigma\sigma'}$$



l = 1 2 3 4

Possible configurations of a single site



$$|0\rangle$$
$$c^\dagger_\uparrow |0\rangle$$
$$c^\dagger_\uparrow c^\dagger_\downarrow |0\rangle$$

Hubbard model -- continued

$$\hat{\mathcal{H}} = \sum_{\substack{\langle ll' \rangle \\ \sigma}} -t \left[\hat{c}^{\dagger}_{l\sigma} \hat{c}_{l'\sigma} + \hat{c}^{\dagger}_{l'\sigma} \hat{c}_{l\sigma} \right] + U \sum_{l} \hat{c}^{\dagger}_{l\uparrow} \hat{c}_{l\uparrow} \hat{c}^{\dagger}_{l\downarrow} \hat{c}_{l\downarrow},$$

t represents electron "hopping" between sites, preserving spin

U represents electron repulsion on a single site

Two-site Hubbard model

$$H = -t\left(c^{\dagger}_{1\uparrow}c_{2\uparrow} + c^{\dagger}_{2\uparrow}c_{1\uparrow} + c^{\dagger}_{1\downarrow}c_{2\downarrow} + c^{\dagger}_{2\downarrow}c_{1\downarrow}\right) + U\left(n_{1\uparrow}n_{1\downarrow} + n_{2\uparrow}n_{2\downarrow}\right)$$

where

$$n_{l\sigma} \equiv c^{\dagger}_{l\sigma}c_{l\sigma}$$

Consider all possible 2 particle states with zero spin:

$$|A\rangle \equiv c^{\dagger}_{1\uparrow}c^{\dagger}_{1\downarrow}|0\rangle$$

$$|B\rangle \equiv c^{\dagger}_{2\uparrow}c^{\dagger}_{2\downarrow}|0\rangle$$

$$|C\rangle \equiv \frac{1}{\sqrt{2}}\left(c^{\dagger}_{1\uparrow}c^{\dagger}_{2\downarrow} - c^{\dagger}_{1\downarrow}c^{\dagger}_{2\uparrow}\right)|0\rangle$$

Two-site Hubbard model

$$H = -t\left(c^{\dagger}_{1\uparrow}c_{2\uparrow} + c^{\dagger}_{2\uparrow}c_{1\uparrow} + c^{\dagger}_{1\downarrow}c_{2\downarrow} + c^{\dagger}_{2\downarrow}c_{1\downarrow}\right) + U\left(n_{1\uparrow}n_{1\downarrow} + n_{2\uparrow}n_{2\downarrow}\right)$$

Matrix elements of Hamiltonian for all 2 particle states with spin 0:

$$H = \begin{pmatrix} U & 0 & -\sqrt{2}t \\ 0 & U & -\sqrt{2}t \\ -\sqrt{2}t & -\sqrt{2}t & 0 \end{pmatrix}$$

Eigenvalues of Hamiltonian:

$$E_1 = -2t\left(\sqrt{1+\left(\frac{U}{4t}\right)^2} - \frac{U}{4t}\right)$$

$$E_2 = U$$

$$E_3 = +2t\left(\sqrt{1+\left(\frac{U}{4t}\right)^2} + \frac{U}{4t}\right)$$

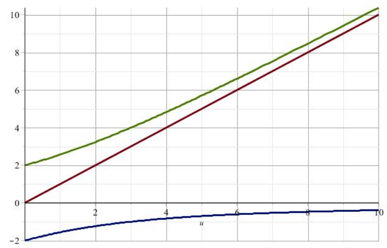
Eigenvectors of the Hamiltonian:

$$|\Psi_1\rangle = \frac{1}{\sqrt{2}}|C\rangle + \frac{1}{2}\left(\sqrt{1+\left(\frac{U}{4t}\right)^2} - \frac{U}{4t}\right)\left(|A\rangle + |B\rangle\right)$$

$$|\Psi_2\rangle = \frac{1}{\sqrt{2}}\left(|A\rangle - |B\rangle\right)$$

$$|\Psi_3\rangle = \frac{1}{\sqrt{2}}|C\rangle - \frac{1}{2}\left(\sqrt{1+\left(\frac{U}{4t}\right)^2} + \frac{U}{4t}\right)\left(|A\rangle + |B\rangle\right)$$

Eigenvalues of the Hubbard model



Eigenvalues of Hamiltonian:

$$E_1 = -2t\left(\sqrt{1+\left(\frac{U}{4t}\right)^2} - \frac{U}{4t}\right)$$

$$E_2 = U$$

$$E_3 = +2t\left(\sqrt{1+\left(\frac{U}{4t}\right)^2} + \frac{U}{4t}\right)$$

Two-site Hubbard model

$$H = -t\left(c^\dagger_{1\uparrow}c_{2\uparrow} + c^\dagger_{2\uparrow}c_{1\uparrow} + c^\dagger_{1\downarrow}c_{2\downarrow} + c^\dagger_{2\downarrow}c_{1\downarrow}\right) + U\left(n_{1\uparrow}n_{1\downarrow} + n_{2\uparrow}n_{2\downarrow}\right)$$

Ground state of the two-site Hubbard model

$$E_1 = -2t\left(\sqrt{1+\left(\frac{U}{4t}\right)^2} - \frac{U}{4t}\right) \qquad |\Psi_1\rangle = \frac{1}{\sqrt{2}}|C\rangle + \frac{1}{2}\left(\sqrt{1+\left(\frac{U}{4t}\right)^2} - \frac{U}{4t}\right)\left(|A\rangle + |B\rangle\right)$$

Single particle limit ($U \rightarrow 0$)

$$E_1 = -2t \qquad |\Psi_1\rangle = \frac{1}{\sqrt{2}}|C\rangle + \frac{1}{2}\left(|A\rangle + |B\rangle\right)$$

$$|A\rangle \equiv c^\dagger_{1\uparrow}c^\dagger_{1\downarrow}|0\rangle \qquad |B\rangle \equiv c^\dagger_{2\uparrow}c^\dagger_{2\downarrow}|0\rangle$$

$$|C\rangle \equiv \frac{1}{\sqrt{2}}\left(c^\dagger_{1\uparrow}c^\dagger_{2\downarrow} - c^\dagger_{1\downarrow}c^\dagger_{2\uparrow}\right)|0\rangle$$