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

Plan for Lecture 34:

- The Hubbard model
  - Linear chain
  - Hartree-Fock approximation
  - “Broken symmetry” solutions
  - LDA+U methods

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	Chap. 26	The Hubbard Model		
34	Mon: 04/20/2015	Chap. 26	The Hubbard Model		
35	Wed: 04/22/2015	Chap. 26	The Hubbard Model		
36	Fri: 04/24/2015		Review		
	Mon: 04/27/2015		Presentations I		
	Wed: 04/29/2015		Presentations II		
	Fri: 05/01/2015		Presentations III & Take home exam		

In the following slides, *u* represents *U/t*:

1d Hubbard Model

Simple Hartree Fock approximation

$$\bar{\mathcal{H}} = -\sum_{n\sigma} \left(C^{\dagger}_{n\sigma} C_{n+1\sigma} + C^{\dagger}_{n\sigma} C_{n-1\sigma} \right) + u \sum_{n} N_{n\uparrow} N_{n\downarrow}. \qquad (12)$$

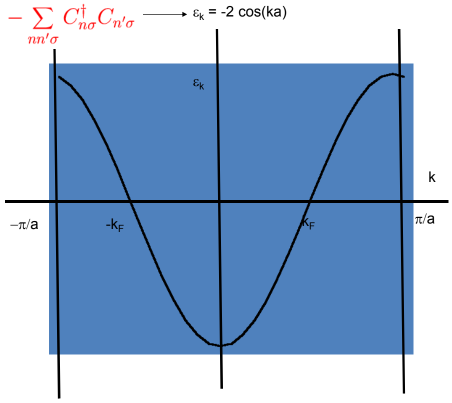
It is convenient to represent the site basis operators $C_{n\sigma}$ in terms of Bloch basis operators $A_{k\sigma}$:

$$A_{k\sigma} \equiv \frac{1}{\sqrt{\mathcal{N}}} \sum_{n} e^{ikan} C_{n\sigma}, \qquad (13)$$

where $\mathcal{N}$ represents the number of lattice sites. In the simple Hartree Fock approximation we assume that $\langle N_{n\uparrow} \rangle = \langle N_{n\downarrow} \rangle = \frac{\mathcal{N}}{2}$ so that where the wavevector k is assumed to take the values $-k_F \le k \le k_F$ and the Fermi wavevector is determined from:

$$2 \sum_{-k_F \le k \le k_F} = \mathcal{N} \;\rightarrow\; k_F = \frac{\pi}{2a}. \qquad (14)$$

$$\bar{\mathcal{H}} = -\sum_{nn'\sigma} C^\dagger_{n\sigma} C_{n'\sigma} \longrightarrow \varepsilon_k = -2\cos(ka)$$



In the *k*-basis, the Hubbard model takes the form:

$$H = -\sum_{k\sigma} 2\cos(ka) A^\dagger_{k\sigma} A_{k\sigma} + u\frac{1}{2\mathcal{N}} \sum_{kq\sigma k'q'\sigma'} A^\dagger_{k\sigma} A^\dagger_{k'\sigma'} A_{q'\sigma'} A_{q\sigma} \delta(-k-k'+q+q')$$

where the delta function must be satisfied modulo a reciprocal lattice vector $\frac{2\pi}{a}$

Simple Hartree-Fock approximation

$$|\Psi_{HF}\rangle = \prod_{-k_F \le k \le k_F} A^\dagger_{k\uparrow} A^\dagger_{k\downarrow} |0\rangle$$

$$E_{HF} = \langle \Psi_{HF} | H | \Psi_{HF} \rangle$$

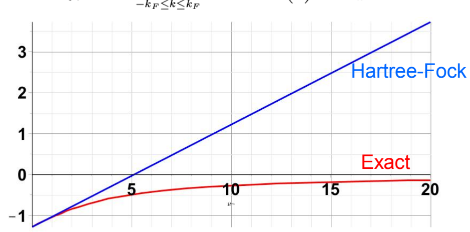
1d Hubbard Model

Simple Hartree Fock approximation (continued)

Evaluating the ground state energy in this simple Hartree Fock approximation, we find that

note that $k_F = \pi/(2a)$

$$\frac{E_{\mathrm{HF}}}{\mathcal{N}} = -4 \sum_{-k_F \le k \le k_F} \cos(ka) + u\left(\frac{1}{2}\right)^2 = -\frac{4}{\pi} + \frac{u}{4}. \qquad (15)$$



One-dimensional Hubbard chain

VOLUME 20, NUMBER 25 PHYSICAL REVIEW LETTERS 17 JUNE 1968

ABSENCE OF MOTT TRANSITION IN AN EXACT SOLUTION OF THE SHORT-RANGE, ONE-BAND MODEL IN ONE DIMENSION

Elliott H. Lieb* and F. Y. Wu
Department of Physics, Northeastern University, Boston, Massachusetts
(Received 22 April 1968)

The short-range, one-band model for electron correlations in a narrow energy band is solved exactly in the one-dimensional case. The ground-state energy, wave function, and the chemical potentials are obtained, and it is found that the ground state exhibits no conductor-insulator transition as the correlation strength is increased.

$$E \equiv E(\tfrac{1}{2}N_a, \tfrac{1}{2}N_a; U)$$
$$= -4N_a \int_0^\infty \frac{J_0(\omega)J_1(\omega)d\omega}{\omega[1+\exp(\tfrac{1}{2}\omega U)]}, \quad (20)$$

In our notation:

$$\frac{E_{exact}}{\mathcal{N}} = -4\int_0^\infty \frac{J_0(w)J_1(w)}{w(1+e^{uw/2})}dw$$

Approximate solutions in terms of single particle states; "broken symmetry" Hartree-Fock type solutions

PHYSICAL REVIEW VOLUME 181, NUMBER 2 10 MAY 1969

Itinerant Antiferromagnetism in an Infinite Linear Chain

B. JOHANSSON AND K-F. BERGGREN
FOA, Fack, Stockholm, Sweden
(Received 30 October 1968)

Overhauser's spin-density-wave state of a general pitch Q is considered for a linear chain with a half-filled band. It is found that $Q=2k_F$ for all values of the coupling constant. Comparison is made with other Hartree-Fock states, and with a recent exact expression for the ground-state energy. The collective modes of the system are calculated numerically, and for large coupling constant they are found to behave as $\omega(q)\sim|\sin(qa)|$.

Broken symmetry Hartree-Fock solution

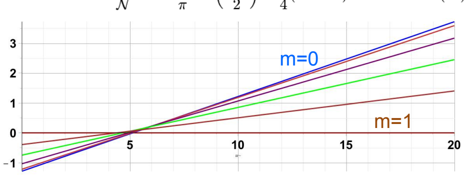
Ferromagnetic Hartree Fock approximation

If we modify the above approach, but allow there to be a different population of up and down spin:

$$\frac{\langle N_{n\uparrow}\rangle - \langle N_{n\downarrow}\rangle}{\langle N_{n\uparrow}\rangle + \langle N_{n\downarrow}\rangle} \equiv m. \quad (16)$$

We find that the Ferromagetic Hartree Fock ground state energy depends on the fractional magnetization m and takes the value:

$$\frac{E_{\rm FHF}}{\mathcal{N}} = -\frac{4}{\pi}\cos\left(\frac{m\pi}{2}\right) + \frac{u}{4}(1-m^2). \quad (17)$$



Spin density wave Hartree Fock approximation

An alternative composite Bloch wave can be defined:

$$S_{k\uparrow} \equiv \cos\theta_k A_{k\uparrow} + \sin\theta_k A_{k+Q\downarrow}. \qquad (26)$$

Here, Q will be determined; for example $Q = \pi / a$ corresponds to a doubled unit cell. (It can be shown that the orthogonal linear combination state does not contribute to the ground state wavefunction.)

$$\left|\Psi_{SDW}\right\rangle = \prod_k S_k^\dagger \left|0\right\rangle$$

$$E_{SDW} = \left\langle \Psi_{SDW}\right| H \left|\Psi_{SDW}\right\rangle = \sum_k E_k^S$$

$$\text{where } E_k^S = \frac{1}{2}\left(\varepsilon_k + \varepsilon_{k+Q}\right) - \frac{1}{2}\left(\left(\varepsilon_k - \varepsilon_{k+Q}\right)^2 + \Delta^2\right)^{1/2}$$

Here $\varepsilon_k = -2\cos(ka)$

Spin density wave solution -- continued

Consistency conditions on Δ:

$$\frac{1}{\mathcal{N}}\sum_k \frac{1}{\left(\left(\varepsilon_k - \varepsilon_{k+Q}\right)^2 + \Delta^2\right)^{1/2}} = \frac{1}{u}$$

$$\tan(2\theta_k) = \frac{\Delta}{\varepsilon_k - \varepsilon_{k+Q}}$$

Expression for energy:

$$\frac{E_{SDW}}{\mathcal{N}} = \frac{1}{2\mathcal{N}}\sum_k \left\{\left(\varepsilon_k + \varepsilon_{k+Q}\right) + \left(\varepsilon_k - \varepsilon_{k+Q}\right)\cos(2\theta_k)\right\} + \frac{u}{4}\left(1 - \frac{1}{\mathcal{N}^2}\sum_{kq}\sin(2\theta_k)\sin(2\theta_q)\right)$$

Johannson and Berggren show that:

$$\eta K(\eta) = \frac{2\pi}{u}\sin(Qa/2)$$

$$\text{where} \quad \eta = \frac{1}{\left(1 + \frac{\Delta^2}{16}\sin^2\left(Qa/2\right)\right)^{1/2}}$$

Elliptic integral:

$$K(m) \equiv \int_0^{\pi/2} \frac{d\phi}{\left(1 - m\sin^2\phi\right)^{1/2}}$$

Spin density wave solution -- continued

Expression for energy:

$$\frac{E_{SDW}}{\mathcal{N}} = -\frac{4}{\pi}\sin(Qa/2)\frac{E(\eta)}{\eta} + \frac{u}{4}\left(1 + \frac{\Delta^2}{u^2}\right)$$

Elliptic integral:

$$E(m) \equiv \int_0^{\pi/2}\left(1 - m\sin^2\phi\right)^{1/2} d\phi$$

Optimal solution obtained for $Qa/2 = \pi/2$:

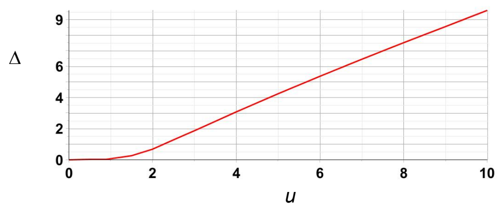
$$\eta K(\eta) = \frac{2\pi}{u} \qquad \text{where} \quad \eta = \frac{1}{\left(1 + \frac{\Delta^2}{16}\right)^{1/2}}$$

$$\frac{E_{SDW}}{\mathcal{N}} = -\frac{4}{\pi}\frac{E(\eta)}{\eta} + \frac{u}{4}\left(1 + \frac{\Delta^2}{u^2}\right)$$

Spin density wave solution -- continued

Numerical solutions for Δ:

$$\frac{2\pi}{\eta K(\eta)} = u \qquad \text{where} \quad \eta = \frac{1}{\left(1+\frac{\Delta^2}{16}\right)^{1/2}}$$



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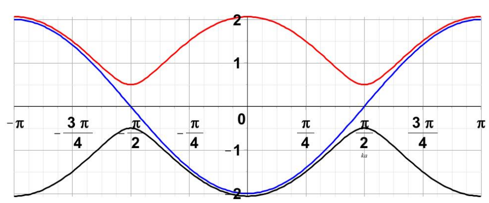
Spin density wave solution -- continued

Effects on single particle states

Non-interacting states: $\varepsilon_k = -2\cos(ka)$

Spin density wave states: $E_k^S = -\frac{1}{2}\left(\left(4\cos(ka)\right)^2 + \Delta^2\right)^{1/2}$



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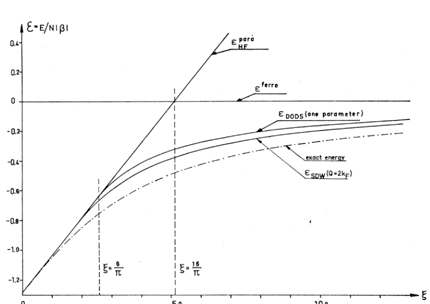
Spin density wave solution -- continued

Nature of spin density wave state:

$S_k = \cos\theta_k A_{k\uparrow} + \sin\theta_k A_{k+\frac{\pi}{a}\downarrow}$

$$\tan(2\theta_k) = \frac{\Delta}{\varepsilon_k - \varepsilon_{k+Q}} = -\frac{\Delta}{4\cos(ka)}$$



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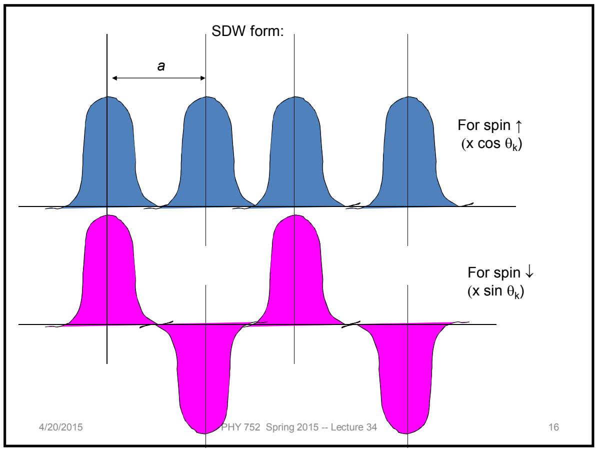
SDW form:
a
For spin ↑
(x cos θk)
For spin ↓
(x sin θk)
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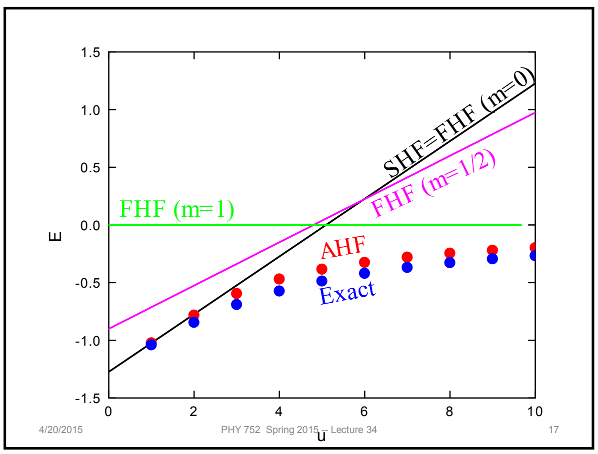
E
u
SHF=FHF (m=0)
FHF (m=1/2)
FHF (m=1)
AHF
Exact
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