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

Plan for Lecture 33:

- **The Hubbard model**
  - **Analysis of solution for a 2 site system**
  - **Hartree-Fock approximation**
  - **Extension to linear chain**

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	Chap. 26	The Hubbard Model		
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		

The Hubbard Hamiltonian:

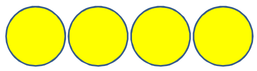
$$\hat{\mathcal{H}} = \sum_{\substack{\langle ll' \rangle \\ \sigma}} -t\left[\hat{c}^{\dagger}_{l\sigma}\hat{c}_{l'\sigma} + \hat{c}^{\dagger}_{l'\sigma}\hat{c}_{l\sigma}\right] + U\sum_{l}\hat{c}^{\dagger}_{l\uparrow}\hat{c}_{l\uparrow}\hat{c}^{\dagger}_{l\downarrow}\hat{c}_{l\downarrow},$$

single particle contribution — two particle contribution

$$\{c_{l\sigma}, c_{l'\sigma'}\} = 0$$

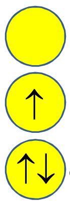
$$\{c^{\dagger}_{l\sigma}, c^{\dagger}_{l'\sigma'}\} = 0$$

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



l = 1 2 3 4

Possible configurations on a single site



$|0\rangle$

$c_\uparrow^\dagger|0\rangle$

$c_\uparrow^\dagger c_\downarrow^\dagger|0\rangle$

Hubbard model -- continued

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

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:

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

$$E_2 = U$$

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

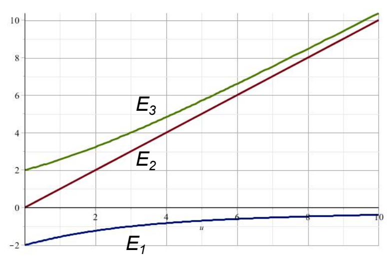
Eigenvectors of the Hamiltonian:

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

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

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

Eigenvalues of the Hubbard model



Eigenvalues of Hamiltonian:

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$$E_2 = U$$

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

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 ($U \rightarrow 0$)

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

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

$$\Rightarrow |\Psi_1\rangle = \frac{1}{2}\left(c^\dagger_{1\uparrow} + c^\dagger_{2\uparrow}\right)\left(c^\dagger_{1\downarrow} + c^\dagger_{2\downarrow}\right)|0\rangle$$

Two-site Hubbard model Single particle limit ($U \rightarrow 0$)

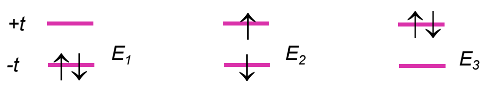
Full spectrum for spin 0 eigenstates

$$E_1 = -2t \qquad |\Psi_1\rangle = \frac{1}{2}\left(c^\dagger_{1\uparrow} + c^\dagger_{2\uparrow}\right)\left(c^\dagger_{1\downarrow} + c^\dagger_{2\downarrow}\right)|0\rangle$$

$$E_2 = 0 \qquad |\Psi_2\rangle = \frac{1}{4}\left(c^\dagger_{1\uparrow} + c^\dagger_{2\uparrow}\right)\left(c^\dagger_{1\downarrow} - c^\dagger_{2\downarrow}\right)|0\rangle + \frac{1}{4}\left(c^\dagger_{1\uparrow} - c^\dagger_{2\uparrow}\right)\left(c^\dagger_{1\downarrow} + c^\dagger_{2\downarrow}\right)|0\rangle$$

$$E_3 = +2t \qquad |\Psi_1\rangle = \frac{1}{2}\left(c^\dagger_{1\uparrow} - c^\dagger_{2\uparrow}\right)\left(c^\dagger_{1\downarrow} - c^\dagger_{2\downarrow}\right)|0\rangle$$

Single particle picture:



Two-site Hubbard model -- Hartree-Fock approximation

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

Wave function assumed to be product of single particle states

Zero order approximation:

Define: $a^\dagger_\sigma \equiv \frac{1}{\sqrt{2}}\left(c^\dagger_{1\sigma} + c^\dagger_{2\sigma}\right)$

Let $\left|\Psi_1^{HF}\right\rangle = a^\dagger_\uparrow a^\dagger_\downarrow |0\rangle$

$$E_1^{HF} = \left\langle \Psi_1^{HF} \middle| H \middle| \Psi_1^{HF} \right\rangle = -2t + \frac{1}{2}U$$

Two-site Hubbard model -- Hartree-Fock approximation

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

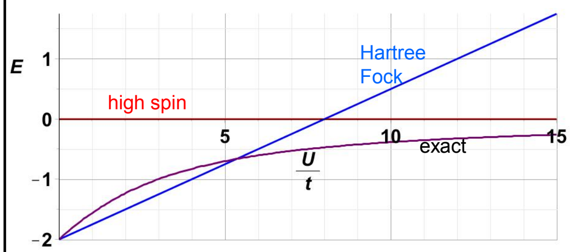
Variational search for lower energy solutions

High spin solution

Let $\left|\Psi_1^{Spin}\right\rangle = c^\dagger_{1\uparrow}c^\dagger_{2\uparrow}|0\rangle$

$E_1^{Spin} = \left\langle \Psi_1^{Spin} \middle| H \middle| \Psi_1^{Spin} \right\rangle = 0$

Ground state energy for 2-site Hubbard model



Two-site Hubbard model -- continued

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

Ground state of the two-site Hubbard model

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

Isolated particle limit ($t \rightarrow 0$)

$$E_1 \approx \frac{-4t^2}{U}$$

$$|\Psi_1\rangle \approx \frac{1}{2}\left(c^\dagger_{1\uparrow}c^\dagger_{2\downarrow} + c^\dagger_{2\uparrow}c^\dagger_{1\downarrow}\right)|0\rangle + \frac{t}{U}\left(c^\dagger_{1\uparrow}c^\dagger_{1\downarrow} + c^\dagger_{2\uparrow}c^\dagger_{2\downarrow}\right)|0\rangle$$

One-dimensional Hubbard chain

VOLUME 20, NUMBER 25 PHYSICAL REVIEW LETTERS 17 JUNE 196[illegible]

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.

$$E \equiv E(\tfrac{1}{2}N_a, \tfrac{1}{2}N_a; U)$$

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

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 $\omega(q)\sim|\sin(qa)|$.

181 ITINERANT ANTIFERROMAGNETISM IN LINEAR CHAIN 857

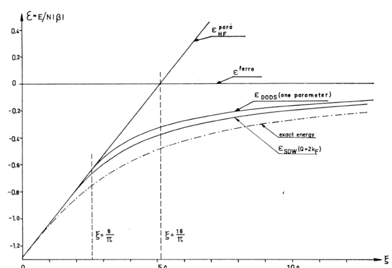


Fig. 2. Total energy per particle in units of $|\beta|$ for different states and approximations as a function of ξ (α is put equal to zero).

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

1d Hubbard Model

Simple Hartree Fock approximation

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

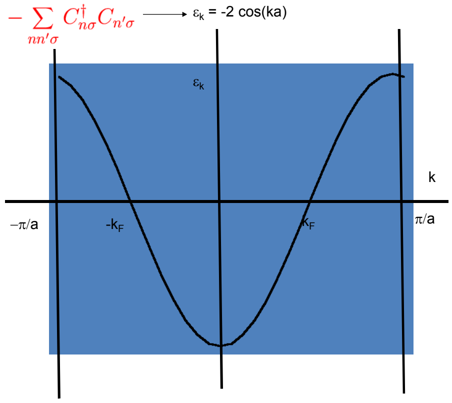
It is convenient to represent the site basis operators $C_{n\sigma}$ in terms of Bloch basis operators $A_{k\sigma}$:

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

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 $-k_F \leq k \leq k_F$ and the Fermi wavevector is determined from:

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

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



1d Hubbard Model

Simple Hartree Fock approximation (continued)

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

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

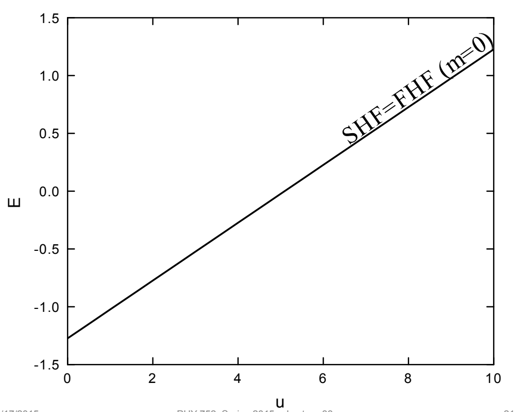
Ferromagnetic Hartree Fock approximation

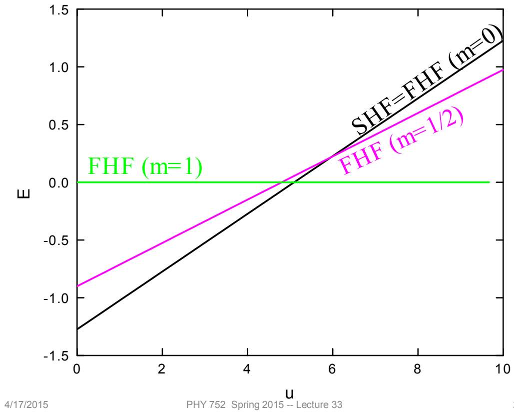
If we modify the above approach, but allow there to be a different population of up and down spin:

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

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

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





1d Hubbard Model

Antiferromagnetic Hartree Fock approximation

Now, we allow the even sites and odd sites to have different spin magnetization: For n even:

$$\langle N_{n\uparrow}\rangle = \frac{1+m}{2} \quad \langle N_{n\downarrow}\rangle = \frac{1-m}{2} \tag{18}$$

and for n odd:

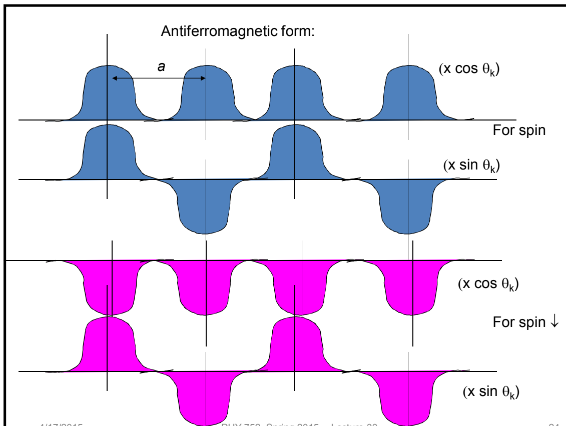
$$\langle N_{n\uparrow}\rangle = \frac{1-m}{2} \quad \langle N_{n\downarrow}\rangle = \frac{1+m}{2}. \tag{19}$$

In this way, the total charge on each site is the same, but the spin magnetization changes sign. Formally, this can be achieved by defining a variational parameter θ_k and defining spin up and spin down composite Bloch waves for the doubled unit cell:

$$D_{k\uparrow} \equiv \cos\theta_k A_{k\uparrow} + \sin\theta_k A_{k+Q\uparrow} \tag{20}$$

$$D_{k\downarrow} \equiv -\cos\theta_k A_{k\downarrow} + \sin\theta_k A_{k+Q\downarrow}, \tag{21}$$

where $Q = \pi/a$.



1d Hubbard Model

Antiferromagnetic Hartree Fock approximation (continued)

We can evaluate the ground state energy as a function of θ_k and then optimize to find the lowest energy. The optimal value of θ_k is found to be given by:

$$\tan 2\theta_k = \frac{um}{4\cos(ka)}. \quad (22)$$

Another relation between m and θ_k comes from the self-consistency condition:

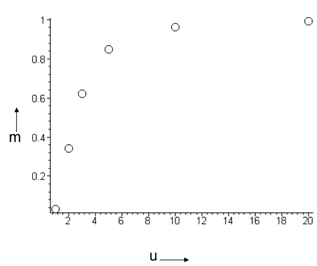
$$\frac{\langle N_{n\uparrow}\rangle - \langle N_{n\downarrow}\rangle}{\langle N_{n\uparrow}\rangle + \langle N_{n\downarrow}\rangle} = m = \sum_k \sin 2\theta_k = \sum_k \frac{um/4}{\sqrt{\cos^2 ka + (um/4)^2}}, \quad (23)$$

which can be put in the form of a transcendental equation:

$$\sqrt{\frac{1}{1+(um/4)^2}}\,K\left(\sqrt{\frac{1}{1+(um/4)^2}}\right) = \frac{2\pi}{u}. \quad (24)$$

For each u, the transcendental equation can be solved for m.

Solutions to AHF equation
for spin magnetization m as a function of u



1d Hubbard Model

Antiferromagnetic Hartree Fock approximation (continued)

The above results then give the calculated ground state energy in the antiferromagnetic Hartree Fock approximation:

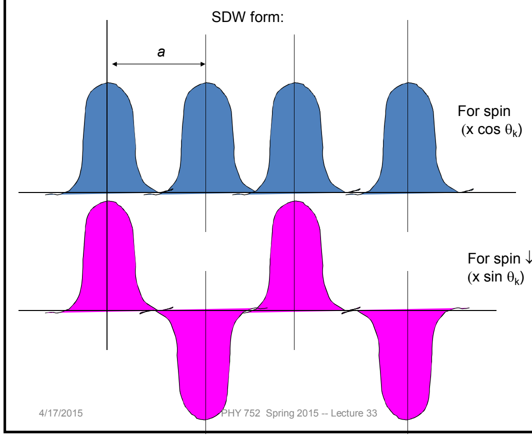
$$\frac{E_{\mathrm{AHF}}}{\mathcal{N}} = -\frac{4}{\pi}\sqrt{1+(um/4)^2}\,E\left(\sqrt{\frac{1}{1+(um/4)^2}}\right) + \frac{u}{4}(1+m^2). \quad (25)$$

Spin density wave Hartree Fock approximation

An alternative composite Bloch wave can be defined:

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

This mixes up and down spin contributions of the Bloch waves and can be shown to have the same ground state energy as that of the antiferromagnetic Hartree Fock solution.



1d Hubbard Model

Spin density wave Hartree Fock approximation (continued)

However, in this case,

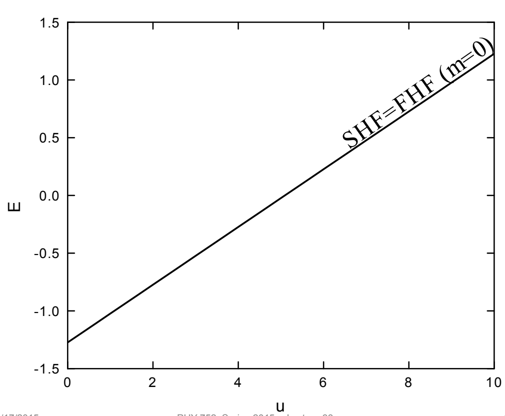
$$\frac{\langle N_{n\uparrow}\rangle - \langle N_{n\downarrow}\rangle}{\langle N_{n\uparrow}\rangle + \langle N_{n\downarrow}\rangle} = 0. \tag{27}$$

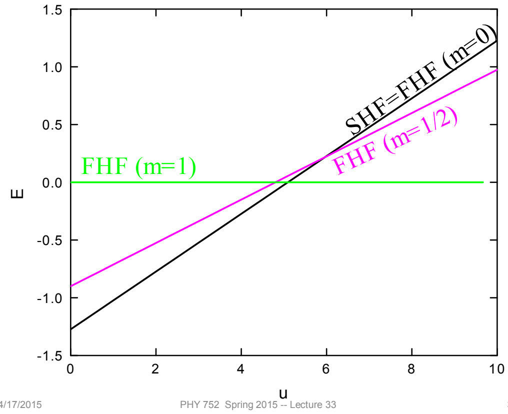
The interpretation of Johansson and Berggren is in terms of spin expection values. For the antiferromagnetic case,

$$\frac{\langle N_{n\uparrow}\rangle - \langle N_{n\downarrow}\rangle}{\langle N_{n\uparrow}\rangle + \langle N_{n\downarrow}\rangle} = \left\langle \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right\rangle = \langle \sigma_z \rangle = \pm m. \tag{28}$$

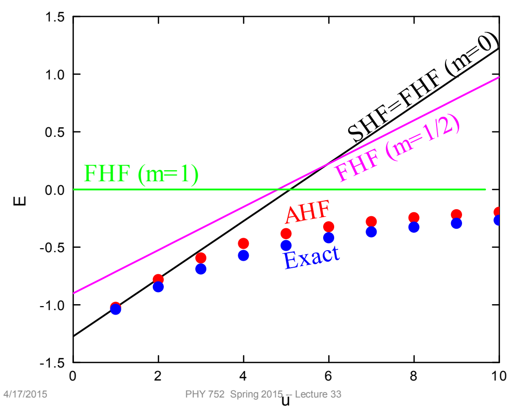
In a similar way, one can show that for the spin density wave case,

$$\left\langle \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \right\rangle = \langle \sigma_x \rangle = \pm m. \tag{29}$$



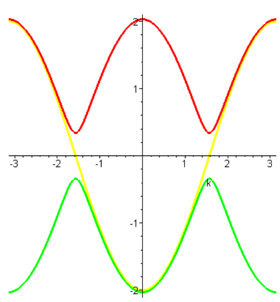


4/17/2015 PHY 752 Spring 2015 -- Lecture 33 31



4/17/2015 PHY 752 Spring 2015 -- Lecture 33 32

Single partical spectra



4/17/2015 PHY 752 Spring 2015 -- Lecture 33 33