PHY 752 Solid State Physics
11-11:50 AM MWF Olin 103

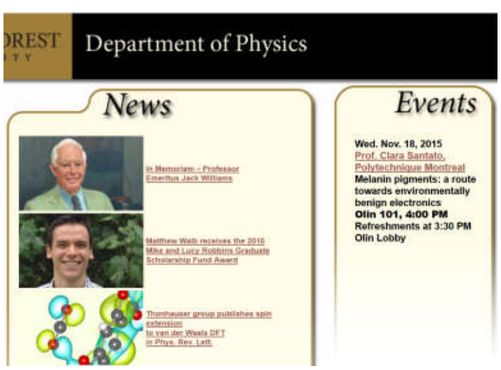
Plan for Lecture 34

Intrinsic spin effects -- Hubbard model

(Chap. 16 & 17 in GGGPP)

1. Exact analysis of 2-site system
2. Periodic one-dimensional system

23	Fri, 10/23/2015	Chap. 11	Optical and transport properties of metals	#21
24	Mon, 10/26/2015	Chap. 11	Optical and transport properties of metals	#22
25	Wed, 10/28/2015	Chap. 11	Transport in metals	#23
26	Fri, 10/30/2015	Chap. 12	Optical properties of semiconductors and insulators	
27	Mon, 11/02/2015	Chap. 7 & 12	Excitons	#24
28	Wed, 11/04/2015	Chap. 9	Lattice vibrations	#25
29	Fri, 11/06/2015	Chap. 9	Lattice vibrations	#26
30	Mon, 11/09/2015	Chap. 13	Defects in semiconductors	#27
31	Wed, 11/11/2015	Chap. 14	Transport in semiconductors	#28
32	Fri, 11/13/2015	Chap. 15	Electron gas in Magnetic fields	#29
33	Mon, 11/16/2015	Chap. 15	Electron gas in Magnetic fields	Prepare presentation.
34	Wed, 11/18/2015	Chap. 17	Magnetic ordering in crystals	Prepare presentation.
35	Fri, 11/20/2015	Chap. 18	Superconductivity	Prepare presentation.
36	Mon, 11/23/2015	Chap. 18	Superconductivity	Prepare presentation.
	Wed, 11/25/2015		*Thanksgiving Holiday*	
	Fri, 11/27/2015		*Thanksgiving Holiday*	
37	Mon, 11/30/2015	Chap. 18	Superconductivity	Prepare presentation.
	Wed, 12/02/2015		Student presentations I	
	Fri, 12/04/2015		Student presentations II	
	Mon, 12/07/2015		Begin Take-home final	



WFU Physics Colloquium

TITLE: Melanin pigments: a route towards environmentally benign electronics

SPEAKER: Professor Clara Santato,

Department of Engineering Physics,
Polytechnique Montreal

TIME: Wednesday November 18, 2015 at 4:00 PM

PLACE: Room 101 Olin Physical Laboratory

efreshments will be served at 3:30 PM in the Olin Lounge. All
iterested persons are cordially invited to attend.

ABSTRACT

Melanins are biomacromolecules responsible for the pigmentation of many plants and animals. The biological functions of melanins, also present in the inner ear and the substantia nigra of the human brain, go far beyond coloration and include photoprotection, anti-oxidant behavior, and metal chelation. Melanins are also intensively studied for their involvement in melanoma skin cancer and Parkinson's disease. In the class of melanins, eumelanins are the most studied by material scientists because of their photoconductivity and hybrid ionic-electronic transport properties.

We will discuss extended structure properties relationships in eumelanins. The film forming properties will be introduced considering their notoriously poorly solubility in all solvents. The interfaces of eumelanin with metals and electrolytes under electrical bias will be critically presented considering the metal binding properties of melanins. The charge transfer and transport properties in different experimental conditions (vacuum vs .wet.) and different electrolytes will be reported.

PHY 752 Presentation Schedule

Wednesday, December 2, 2015

	Presenter	Title of presentation
10:00-10:25	Larry Rush	First Principles Investigation of the geometrical and electrochemical properties of Na4P2S6 and Li4P2S6
10:25-10:50	Katelyn Goetz	Poole-Frenkel Effect in an Ambipolar Material

Friday, December 4, 2015

	Presenter	Title of presentation
10:00-10:25	Gabriel Marcus	Thermoelectric Materials
10:25-10:50	Nathan Beets	Magnetic fields in the Electron Gas

Intrinsic spin of an electron

Magnetic moment of an electron

$$\mu_s = -g_0 \mu_B \mathbf{s}$$

$$\mu_B = \frac{e\hbar}{2mc} = 0.05788 \text{ meV/T}$$

$$\mathrm{g}_0 = 2.0023193043622$$

$$\mathbf{s} = \frac{1}{2}\left(\sigma_x \hat{\mathbf{x}} + \sigma_y \hat{\mathbf{y}} + \sigma_z \hat{\mathbf{z}}\right)$$

Short hand notation for eigenstates σ of σ_z

$$\sigma = +1 \uparrow$$

$$\sigma = -1 \downarrow$$

THE ROYAL SOCIETY PUBLISHING

Electron Correlations in Narrow Energy Bands
Author(s): J. Hubbard
Source: Proceedings of the Royal Society of London. Series A, Mathematical and Physical Sciences, Vol. 276, No. 1365 (Nov. 26, 1963), pp. 238-257
Published by: The Royal Society
Stable URL: http://www.jstor.org/stable/2414761
Accessed: 15-04-2015 03:16 UTC

Electron correlations in narrow energy bands

By J. Hubbard
Theoretical Physics Division, A.E.R.E., Harwell, Didcot, Berks

(*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:

single particle contribution — two particle contribution

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

anti-commutator for Fermi particles

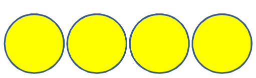
$$\{c_{l\sigma}, c_{l'\sigma'}\} = 0$$

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

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

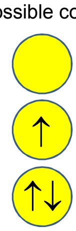
l denotes a site

σ denotes spin ($\uparrow$ or $\downarrow$)



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

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

Note that total spin Σ = 0,1 and the z-component of the total spin Σ_z=-1,0,1 commute with *H* and are good eigenvalues of the states of the system. For Σ = 1, there are 3 values of Σ_z=-1,0,1 which have the same eigenvalues.

For $|\Sigma\Sigma_z\rangle = |11\rangle = \left(c^{\dagger}_{1\uparrow}c^{\dagger}_{2\uparrow}\right)|0\rangle$

Note that: $H|11\rangle = E|11\rangle$ for $E = 0$

Two-site Hubbard model -- continued

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

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:

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

$$E_2 = U$$

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

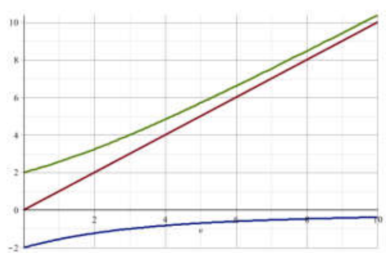
Eigenvectors of the Hamiltonian:

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

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

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

Eigenvalues of the Hubbard model



Eigenvalues of Hamiltonian:

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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 ($U \rightarrow 0$)

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

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

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

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

1d Hubbard Model

Simple Hartree Fock approximation

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

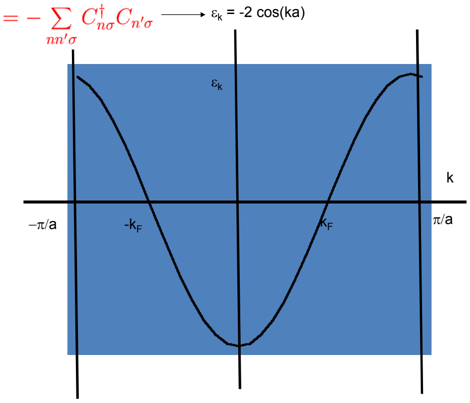
It is convenient to represent the site basis operators $C_{n\sigma}$ in terms of Bloch basis operators $A_{k\sigma}$:

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

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:

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

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



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

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

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

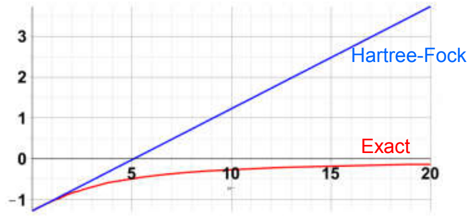
1d Hubbard Model

Simple Hartree Fock approximation (continued)

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

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

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



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.

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

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

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

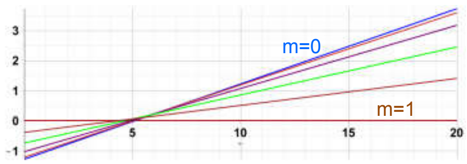
Ferromagnetic Hartree Fock approximation

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

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

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

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



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.)

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

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

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

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:

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

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

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 $Qa/2=\pi/2$:

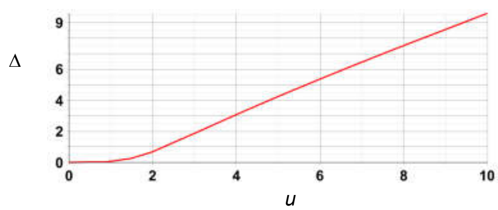
$$\eta K(\eta)=\frac{2\pi}{u} \qquad \text{where} \quad \eta=\frac{1}{\left(1+\frac{\Delta^2}{16}\right)^{1/2}}$$

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

Spin density wave solution -- continued

Numerical solutions for Δ:

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

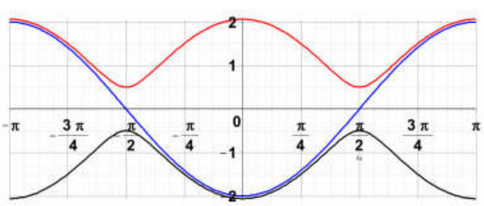


Spin density wave solution -- continued

Effects on single particle states

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

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

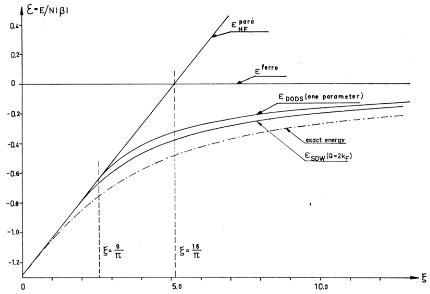


Spin density wave solution -- continued

Nature of spin density wave state:

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

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



SDW form: