

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

Plan for Lecture 12:
Reading: Chapter 9 in MPM
Approximations to the many electron problem -- continued

- 1. Density functional theory**
- 2. Exchange energy and potential for jellium**

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Course schedule for Spring 2015
(Preliminary schedule -- subject to frequent adjustment.)

	Lecture date	MPM Reading	Topic	Assign.	Due date
1	Mon: 01/12/2015	Chap. 1 & 2	Crystal structures	#1	01/23/2015
2	Wed: 01/14/2015	Chap. 1 & 2	Some group theory	#2	01/23/2015
	Fri: 01/16/2015	No class	NAWH out of town		
	Mon: 01/19/2015	No class	MLK Holiday		
3	Wed: 01/21/2015	Chap. 1 & 2	Some group theory	#3	01/23/2015
4	Fri: 01/23/2015	Chap. 1 & 2	Some more group theory	#4	01/28/2015
5	Mon: 01/26/2015	Chap. 7.3	Some more group theory	#5	01/28/2015
6	Wed: 01/28/2015	Chap. 6	Electronic structure; Free electron gas	#6	01/30/2015
7	Fri: 01/30/2015	Chap. 7	Electronic structure; Model potentials	#7	02/02/2015
8	Mon: 02/02/2015	Chap. 8	Electronic structure; LCAO	#8	02/04/2015
9	Wed: 02/04/2015	Chap. 8	Electronic structure; LCAO and tight binding	#9	02/06/2015
10	Fri: 02/06/2015	Chap. 8	Band structure examples	#10	02/09/2015
11	Mon: 02/09/2015	Chap. 9	Electron-electron interactions	#11	02/11/2015
12	Wed: 02/11/2015	Chap. 9	Electron-electron interactions	#12	02/13/2015

Note: Take-home exam scheduled for the week of March 2nd.

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WFU Physics Colloquium

TITLE: Bio-inspired Tensegrity Structures

SPEAKER: Dr. Cornel Sultan,
*Department of Aerospace and Ocean Engineering
Virginia Polytechnic Institute and State University*

TIME: Wednesday February 11, 2015 at 4:00 PM

PLACE: Room 101 Olin Physical Laboratory

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

ABSTRACT

Tensegrity structures are assemblies of stretched tendons and disjoint bars that originated in the abstract art of the 1900s. Today they are perceived as promising structural systems in areas ranging from space applications to bioengineering. In this talk the artistic context of the late 1800s and early 1900s is briefly revisited and tensegrity's invention by artist Kenneth Snelson is discussed.

The presentation then focuses on tensegrity deployment (i.e. how they can be folded/unfolded). A deployment strategy inspired by the way biological organisms control motion via tendons and muscles is presented. First, the equations of motion are derived

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Density functional theory

Describes the relationship between the many electron problem and independent electron treatments.

Proof of theorem

Estimates of $F[n]$.

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Density functional theory -- continued

PHYSICAL REVIEW VOLUME 156, NUMBER 1B 9 NOVEMBER 1964

Inhomogeneous Electron Gas*

D. HOMBERGER
Ecole Normale Supérieure, Paris, France

AND

W. KOHN
Ecole Normale Supérieure, Paris, France and Faculty of Sciences, Orsay, France
and
University of California at San Diego, La Jolla, California
(Received 18 June 1964)

This paper deals with the ground state of an interacting electron gas in an external potential $v(\mathbf{r})$. It is proved that there exists a universal functional of the density, $F[n(\mathbf{r})]$, independent of $v(\mathbf{r})$, such that the expression $E[n(\mathbf{r})] = T[n(\mathbf{r})] + F[n(\mathbf{r})] + \int v(\mathbf{r})n(\mathbf{r})d\mathbf{r}$ has as its minimum value the correct ground-state energy associated with $v(\mathbf{r})$. The functional $F[n(\mathbf{r})]$ is then discussed for two situations: (1) $n(\mathbf{r}) = n_0 + \delta n(\mathbf{r})$, $\delta n_0 < 1$, and (2) $n(\mathbf{r}) = n_0 + \delta n(\mathbf{r})$ with n_0 arbitrary and $\delta n \rightarrow \infty$. In both cases F can be expressed entirely in terms of the correlation energy and linear and higher order electronic polarizabilities of a uniform electron gas. This approach also sheds some light on generalized Thomas-Fermi methods and their limitations. Some new extensions of these methods are presented.

PHYSICAL REVIEW VOLUME 140, NUMBER 4A 15 NOVEMBER 1965

Self-Consistent Equations Including Exchange and Correlation Effects*

W. KOHN AND L. J. SHAM
University of California, San Diego, La Jolla, California
(Received 21 June 1965)

From a theory of Hohenberg and Kohn, approximation methods for treating an inhomogeneous system of interacting electrons are developed. These methods are exact for systems of slowly varying or high density. For the ground state, they lead to self-consistent equations analogous to the Hartree and Hartree-Fock equations, respectively. In these equations the exchange and correlation portions of the chemical potential of a uniform electron gas appear as additional effective potentials. (The exchange portion of our effective potential differs from that due to Slater by a factor of 1/2.) Electronic systems at finite temperatures and in magnetic fields are also treated by similar methods. An appendix deals with a further correction for systems with short-wavelength density oscillations.

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Hohenberg and Kohn: formal proof of basic theorem

The system consists of N electrons interacting via their mutual Coulomb repulsion in the presence of an "external" single particle potential $v(\mathbf{r})$.

$$H = T + V + U$$

Kinetic External Coulomb
energy potential interaction

Consider a many Fermion wavefunction $|\Psi\rangle$.

The (many electron) density can be calculated from $n(\mathbf{r}) = \langle \Psi | \sum_i \delta(\mathbf{r} - \mathbf{r}_i) | \Psi \rangle$

$$= N \int d^3r_1 \dots d^3r_N \Psi^*(r_1, r_2, \dots, r_N) \sum_i \delta(\mathbf{r} - \mathbf{r}_i) \Psi(r_1, r_2, \dots, r_N)$$

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Theorem: The density $n(\mathbf{r})$ of the ground state of the system is a unique functional of the external potential $v(\mathbf{r})$.

Proof: Consider two Hamiltonians H and H' differing only by external potentials v and v' .

Ground state energies: $E = \langle \Psi | H | \Psi \rangle$

and $E' = \langle \Psi' | H' | \Psi' \rangle$

Note that $E' = \langle \Psi' | H' | \Psi' \rangle \leq \langle \Psi' | H | \Psi' \rangle$

$$\begin{aligned} \langle \Psi' | H' | \Psi' \rangle &= \langle \Psi' | H + V' - V | \Psi' \rangle \\ &= \langle \Psi' | H | \Psi' \rangle + \langle \Psi' | V' - V | \Psi' \rangle \\ &= E + \int d^3r n(\mathbf{r})(v'(\mathbf{r}) - v(\mathbf{r})) \\ \Rightarrow E' &\leq E + \int d^3r n(\mathbf{r})(v'(\mathbf{r}) - v(\mathbf{r})) \end{aligned}$$

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We can also show:

$$\begin{aligned} \text{Note that } E &= \langle \Psi | H | \Psi \rangle \leq \langle \Psi' | H | \Psi' \rangle \\ \langle \Psi' | H | \Psi' \rangle &= \langle \Psi' | H' + V - V' | \Psi' \rangle \\ &= \langle \Psi' | H' | \Psi' \rangle + \langle \Psi' | V - V' | \Psi' \rangle \\ &= E' + \int d^3r n'(\mathbf{r})(v(\mathbf{r}) - v'(\mathbf{r})) \\ \Rightarrow E &\leq E' + \int d^3r n'(\mathbf{r})(v(\mathbf{r}) - v'(\mathbf{r})) \\ E' &\leq E + \int d^3r n(\mathbf{r})(v'(\mathbf{r}) - v(\mathbf{r})) \\ E &\leq E' + \int d^3r n'(\mathbf{r})(v(\mathbf{r}) - v'(\mathbf{r})) \\ \Rightarrow n(\mathbf{r}) &\equiv n'(\mathbf{r}) \quad \text{if } v(\mathbf{r}) \equiv v'(\mathbf{r}) \end{aligned}$$

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The theorem implies that the ground state energy E can be considered as a functional of the density $n(\mathbf{r})$

$$E_v[\Psi] = F[n] + \int d^3r v(\mathbf{r}) n(\mathbf{r})$$

Thus, the determination of the ground state energy E is transformed into a minimization of the functional with respect to the density $n(\mathbf{r})$, transforming a many particle minimization into a single particle minimization.

In practice, the functional form of $F[n]$ is not known.

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Determination of $F[n]$ for jellium

Assume we have N particles in a volume \mathcal{V}
with $n = N / \mathcal{V}$:

Kinetic energy contribution:

$$T = \frac{2\mathcal{V}}{(2\pi)^3} \int d^3k \frac{\hbar^2 k^2}{2m} = \frac{2\mathcal{V}}{(2\pi)^3} \frac{\hbar^2}{2m} 4\pi \frac{k_F^5}{5}$$

Recall that $k_F = (3\pi^2 n)^{1/3}$

$$\Rightarrow T = \frac{\hbar^2 \mathcal{V}}{2m} \frac{3}{5} (3\pi^2)^{2/3} n^{5/3}$$

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Determination of $F[n]$ for jellium -- continued

The Coulomb (Hartree) contribution:

$$E_{ee} = \frac{e^2}{2} \int d^3r \int d^3r' \frac{n(\mathbf{r})n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|}$$

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Determination of $F[n]$ for jellium – continued
Exchange contribution within Hartree-Fock approximation

Previously we have shown:

$$E_{ex} = -\frac{e^2}{2} \sum_{i,j} \delta_{\sigma_i \sigma_j} \int d^3r \phi_{n, \mathbf{k}_i, \sigma_i}^*(\mathbf{r}) \phi_{n, \mathbf{k}_j, \sigma_j}(\mathbf{r}) \int d^3r' \frac{\phi_{n, \mathbf{k}_j, \sigma_j}^*(\mathbf{r}') \phi_{n, \mathbf{k}_i, \sigma_i}(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|}$$

For jellium:

$$\phi_{n, \mathbf{k}_j, \sigma_j}(\mathbf{r}) = \frac{1}{\sqrt{\mathcal{V}}} e^{i\mathbf{k}_j \cdot \mathbf{r}}$$

It can be shown that

$$E_{ex} = -\frac{2\mathcal{V}e^2 k_F^4}{(2\pi)^3} = -\frac{2\mathcal{V}e^2 (3\pi^2 n)^{4/3}}{(2\pi)^3} = -\frac{3\mathcal{V}e^2 n}{4\pi} (3\pi^2 n)^{1/3}$$

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Summary of results for jellium:

$$E_v[\Psi] \equiv E_v[n] = F[n] + \int d^3r v(\mathbf{r}) n(\mathbf{r})$$

$$E_v[n] = T[n] + E_{ee}[n] + E_{ex}[n] + E_{ext}[n]$$

$$E_{ext}[n] \equiv \int d^3r v(\mathbf{r}) n(\mathbf{r})$$

$$E_{ee} = \frac{e^2}{2} \int d^3r \int d^3r' \frac{n(\mathbf{r})n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|}$$

} General forms

$$T[n] = \frac{\hbar^2 \mathcal{V}}{2m} \frac{3}{5} (3\pi^2)^{2/3} n^{5/3}$$

} Special for jellium

$$E_{ex}[n] = -\frac{3\mathcal{V}e^2 n}{4\pi} (3\pi^2 n)^{1/3}$$

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Variational equations

$$\frac{\partial E_v[n]}{\partial \delta n} = 0$$

Constraint on density:

$$N[n] = \int d^3r n(\mathbf{r}) = N$$

$$\text{Let } n(\mathbf{r}) = \sum_i |\phi_i(\mathbf{r})|^2$$

Resulting equations for orbitals $\phi_i(\mathbf{r})$:

$$\left(-\frac{\hbar^2}{2m} \nabla^2 + V_{ee}(\mathbf{r}) + V_{ex}(\mathbf{r}) + v(\mathbf{r}) \right) \phi_i(\mathbf{r}) = \epsilon_i \phi_i(\mathbf{r})$$

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Summary of Kohn-Sham equations:

$$\text{Let } n(\mathbf{r}) = \sum_i |\phi_i(\mathbf{r})|^2$$

Resulting equations for orbitals $\phi_i(\mathbf{r})$:

$$\left(-\frac{\hbar^2}{2m} \nabla^2 + V_{ee}(\mathbf{r}) + V_{ex}(\mathbf{r}) + v(\mathbf{r}) \right) \phi_i(\mathbf{r}) = \epsilon_i \phi_i(\mathbf{r})$$

$$V_{ee}(\mathbf{r}) = e^2 \int d^3r' \frac{n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|}$$

$$V_{ex}(\mathbf{r}) = -\frac{e^2}{\pi} (3\pi^2 n)^{1/3} \quad \text{For jellium; exchange only}$$

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