LECTURE # 29 e Title	4/1/2009
	INTRODUCTION
Quantum Hall effect Graphene	TO DENSITY
Carbon Nanotubes	FUNCTIONAL THEORY
Excitons and exciton-polaritons	
Mesoscopic physics and single electronics Spectroscopy of quantum dots and quantum wires	HARTREE - FOCK
Spintronics in metals/semiconductors	
Neutron and electron scattering in solids	
Solid state devices for quantum information processing	/ E [ ? Y, Y, Z ( -> Functional
Magnetic properties of solids	
Superconductivity	

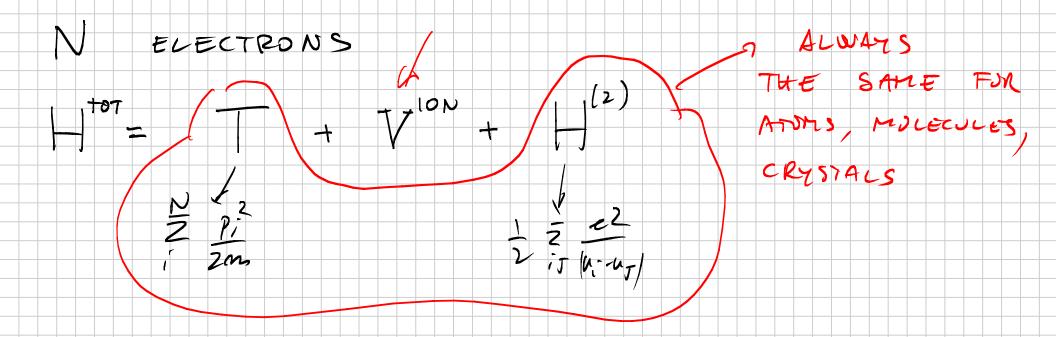
#### ScHR Y. EFFECTIVE PARTICLE Đ 1 Ð SY:\*

0

HARTREE  $\mathbf{+}$ EXCHANGE

FUNCTIONAL DENSITY 1

 $\int m(n)$ FUNCTION AL 727 AS ENERGY SP VARIATION E/M(n)0 8 (EZECTONIC DENSITY) ON MA) M(u)SM



ALL PROPERTIES OF N-ELECTRON SYSTEMS

ARE UNIQUELY DETERMINED BY VENU

ANY OBSERVABLE O[v(u)] is

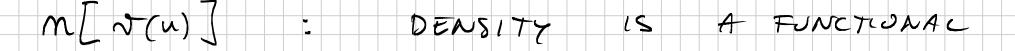
A FUNCTIONAL OF NOW)

1

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IN PARTICULAR, TOTAL DENSITY

DI UMANY-BUDY < UMANY - BUDY  $Z \delta(n-n;)$  $\hat{\rho} =$ 2 = m(n)

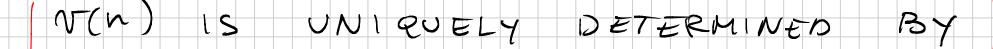


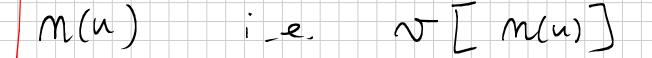
OF V(U)

### DENSITY FUNCTIONAL THEORY BASED ON

9 -

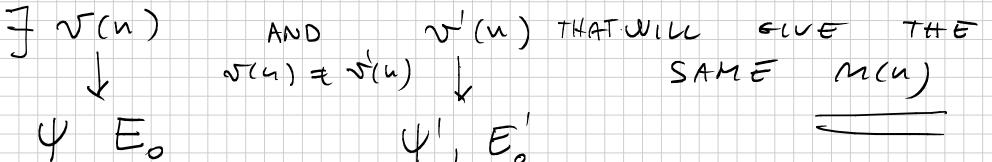
# HOHENBERG-KOHN THEOREM:





REDUCTIO AD ABSUROUM:

IFSTATEMENT UP THEOREM IS NOT TRUE THEN



THEN

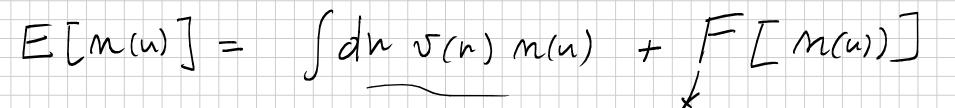
 $E_{o} = \angle \psi | T + v + H^{2} | \psi \rangle \langle \angle \psi | T + v + H^{2} | \psi \rangle = + v' - v'$  $(4'|T+v'+H^2+v-v'|4') = E_0' + (4'|v-v'|4')$  $E_{o} - E_{o} < \int dr m(u) (N(u) - N(u))$  (a)  $E_{0}^{\prime} = 2 \psi^{\prime} | T + v^{\prime} + t \psi^{2} | \psi^{\prime} \rangle < 2 \psi^{\prime} | T + v^{\prime} + t \psi^{2} | \psi^{2} \rangle$  $= \frac{1}{2} = \frac{1}{2} = \frac{1}{2} \int dn m(n) \left( \nabla(n) - \nabla'(n') \right) \quad (b)$  $(\alpha) + (b)$  ARE TRUE ONLY IF V(n) = v(n)ABSURDUM  $\langle \mathcal{U} | \hat{\rho} | \mathcal{U} \rangle = \langle \mathcal{U} | \rho | \mathcal{U} \rangle$ M(n) =

-> ELVIMJ => E[V(u)]

GROUND STATE MANY BODY ENER 64 3 / M(u)

# UNIQUELY DETERMINED BY MU

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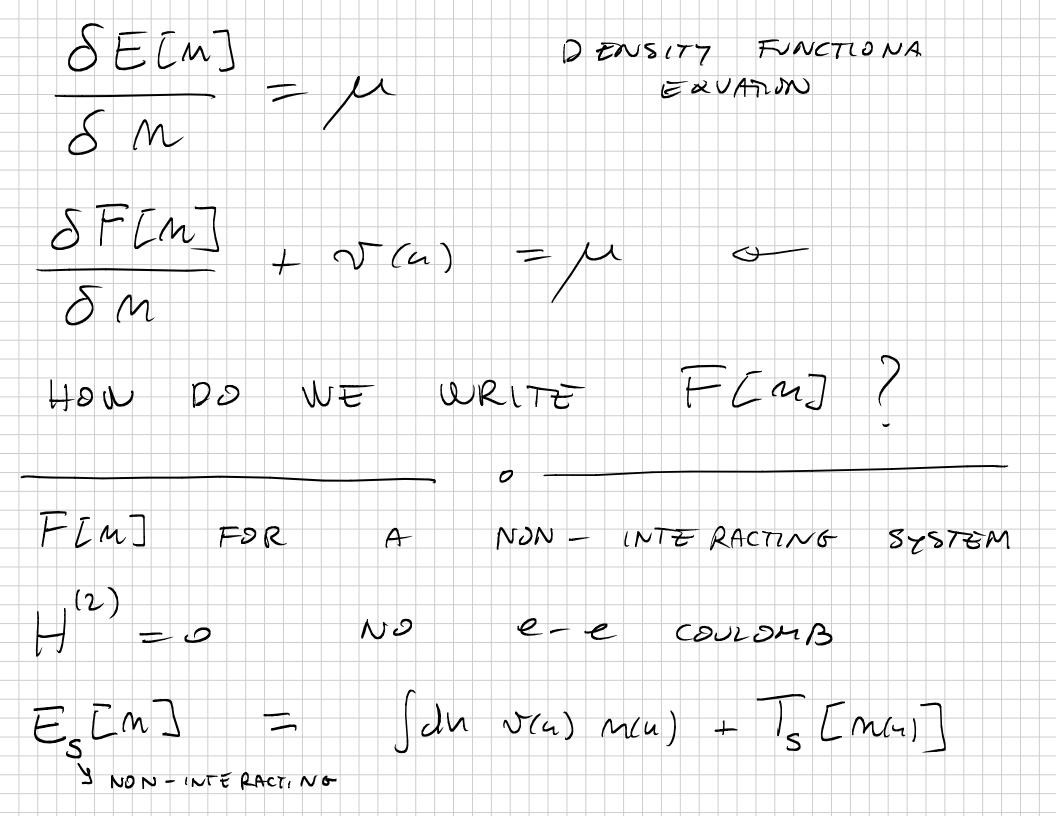


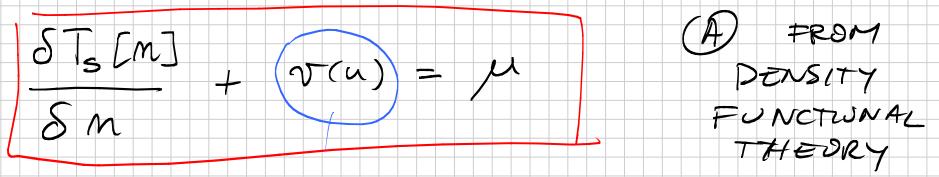
KINETIC TERM +

COULDAB

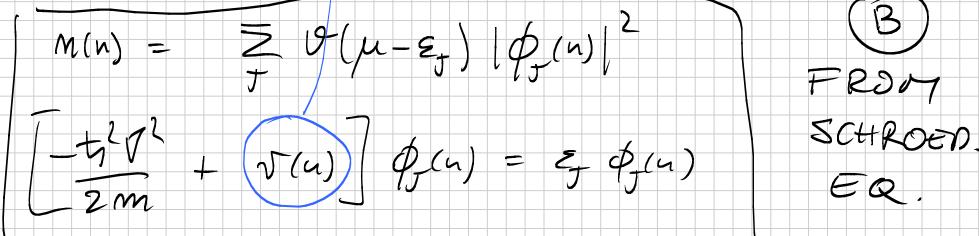
VARIATIONAL METHOD

 $S(EIm] - \mu (dn M(n))$  $\mathcal{O}$ 





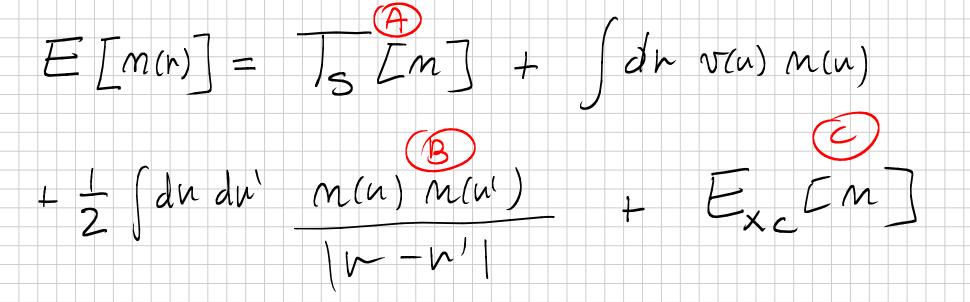
### EQUIVALENT TO:



## THIS LINK BETWEEN SE AND

DFT IS USED IN THE

SHAM EQUATIONS OHN

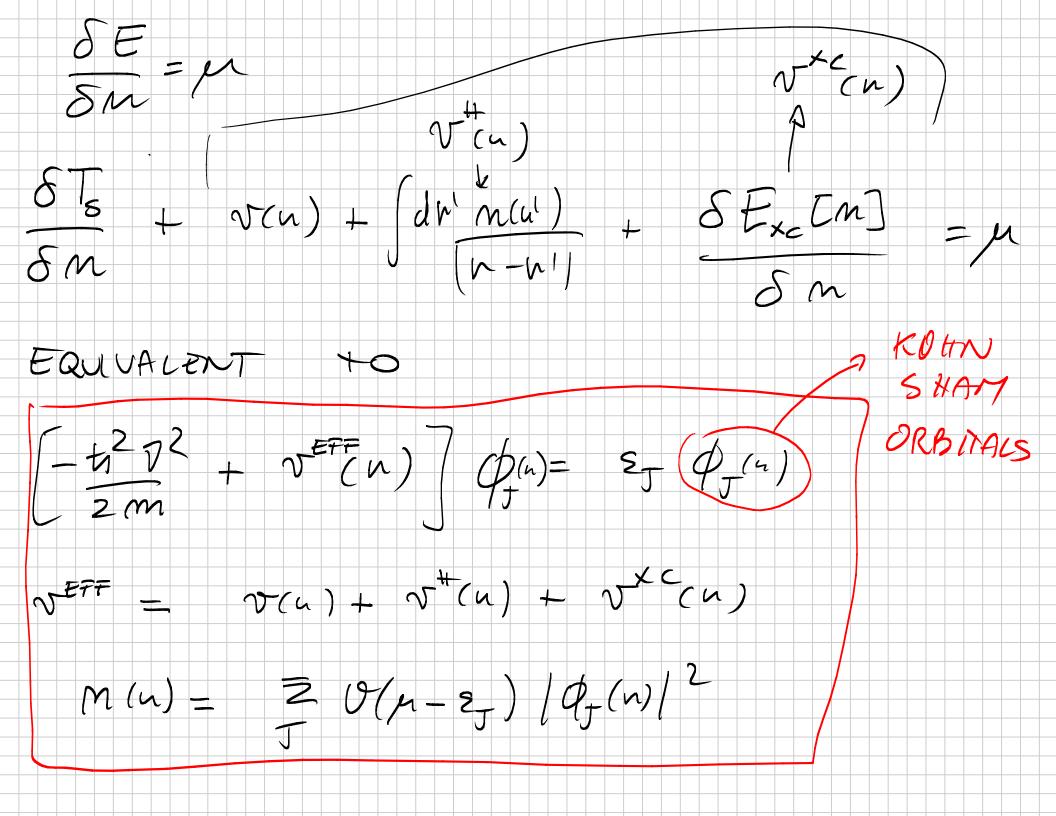


IS [M] KINETIC ENERGY UF NOW-INTERACTIVE

SYSTEM WITH SAME DENSITY M(n)

HARTREE

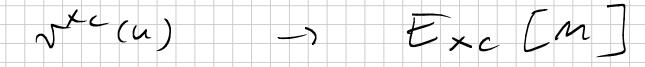
EXCHANGE - CORRECATION



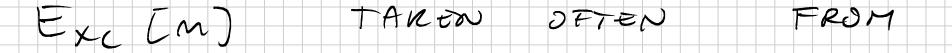
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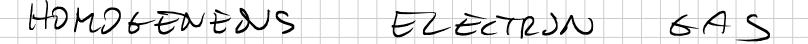


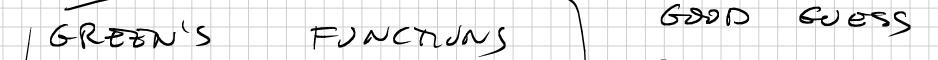
UHAT IS IN NECCH)



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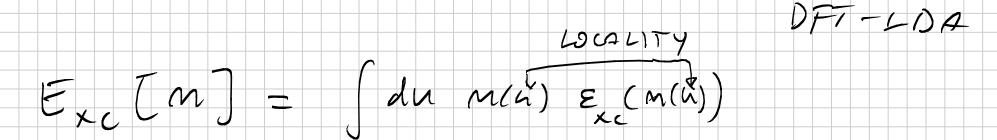




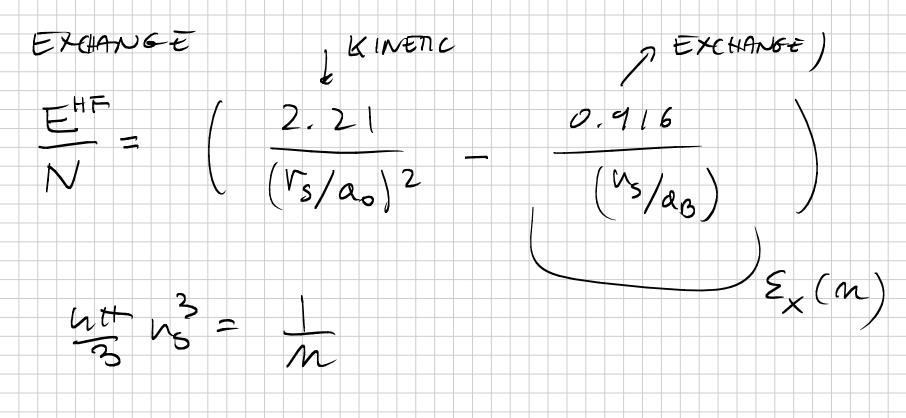


QUANTIM MONTECARLO / Exc





### YOU COULD USE HUMEGAS + HF FOR THE



 $z_x(m) = -\alpha m^3$ 

 $E^{\star c}$   $TmJ = - \alpha \int dn m(n) m^{\prime 3}(n)$ 

