Title: Explorations in Condensed Matter-5

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URL: http://pirsa.org/15030038

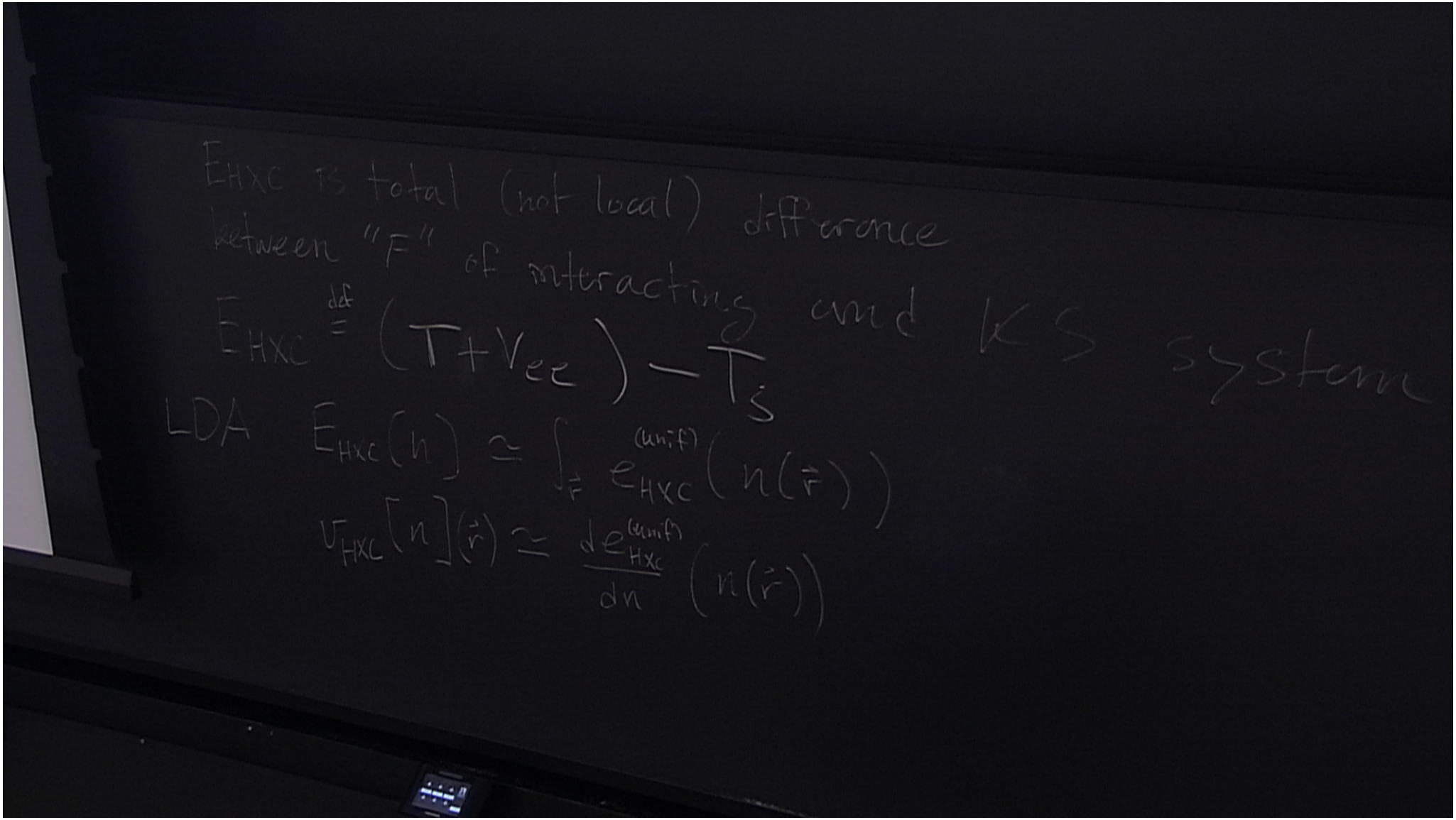
Abstract:

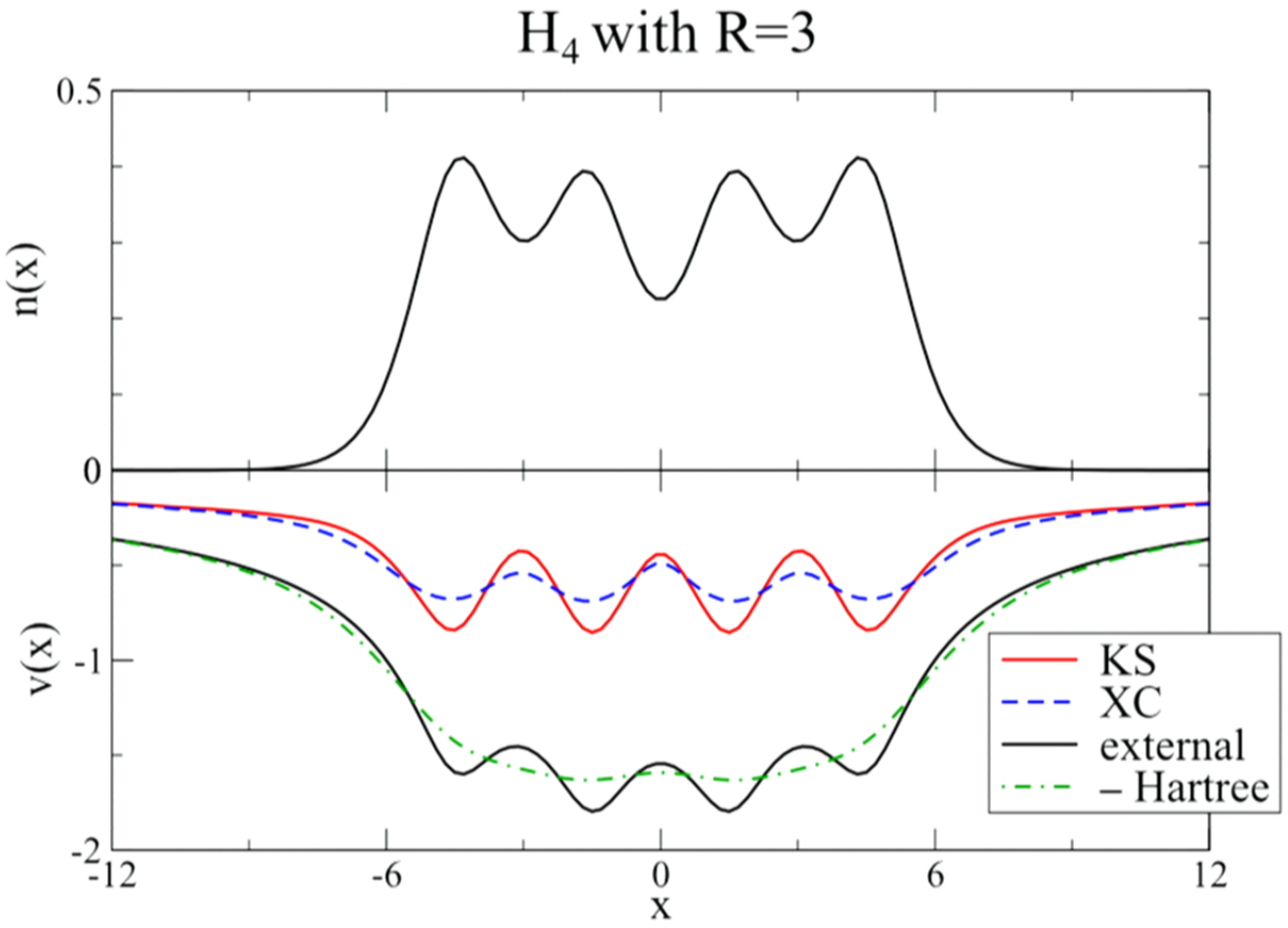
$$E[n] = \underbrace{T[n] + V_{ee}[n]}_{F[n]} + \int v(\vec{r})\, n(\vec{r})$$

$$\overset{(def)}{=} T_s[n] + E_{HXC}[n] + \int v(\vec{r})\, n(\vec{r})$$

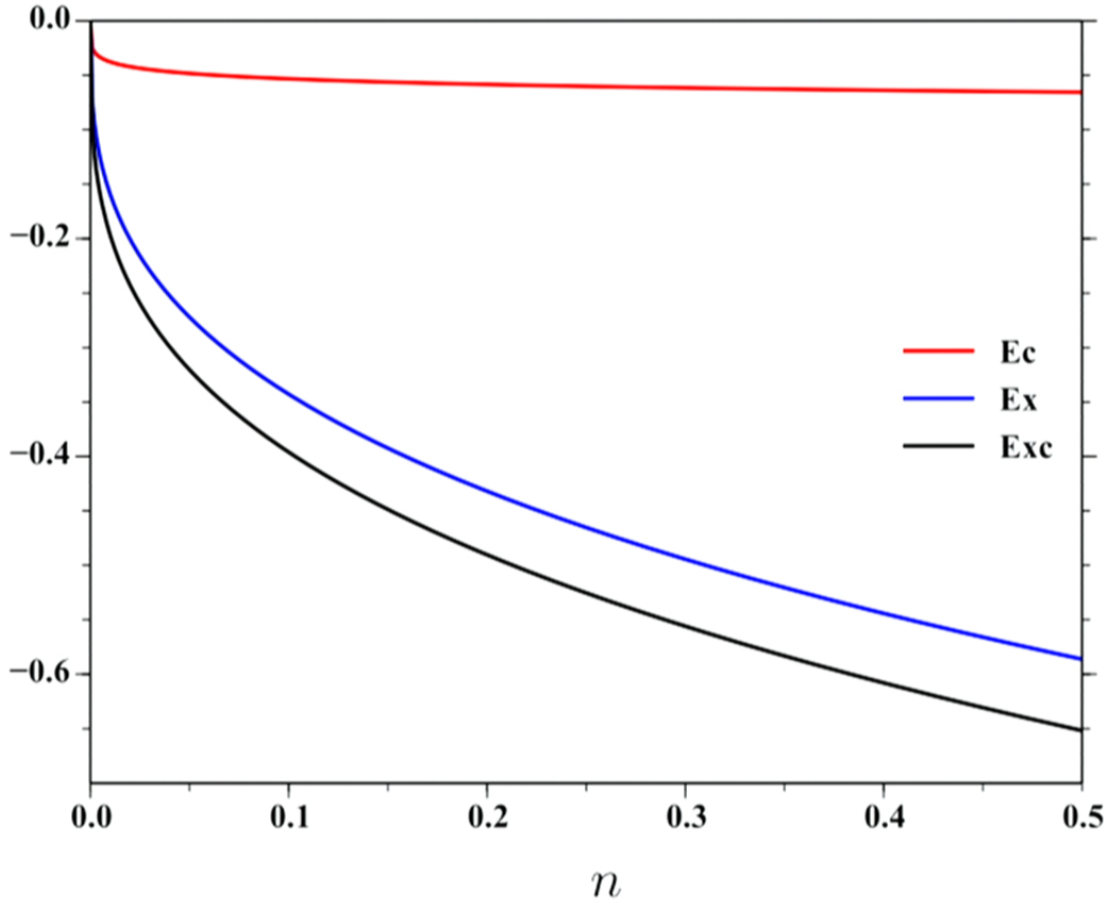
$$\left.\frac{\delta E[n]}{\delta n}\right|_{n=n_0} = 0 \overset{(def)}{=} -v_s(\vec{r}) + v_{HXC}(\vec{r}) + v(\vec{r})$$

$$\Rightarrow v_s(\vec{r}) = v(\vec{r}) + v_{HXC}(\vec{r})$$


E_{HXC} is total (not local) difference between "F" of interacting and KS system
$E_{HXC} \overset{df}{=} (T + V_{ee}) - T_s$
LDA $E_{HXC}(n) \simeq \int_{\vec{r}} e_{HXC}^{(unif)}(n(\vec{r}))$
$v_{HXC}[n](\vec{r}) \simeq \frac{de_{HXC}^{(unif)}}{dn}(n(\vec{r}))$


H_4 with R=3
0.5
0
n(x)
-1
-2
v(x)
-12
-6
0
6
12
x
KS
XC
external
– Hartree

Fit of 3d Coulomb exchange-correlation energy (per electron)



Perdew, Wang PRB (1992) - cited over 10,000 times!

KS algorithm

1. Solve i^{th} KS system

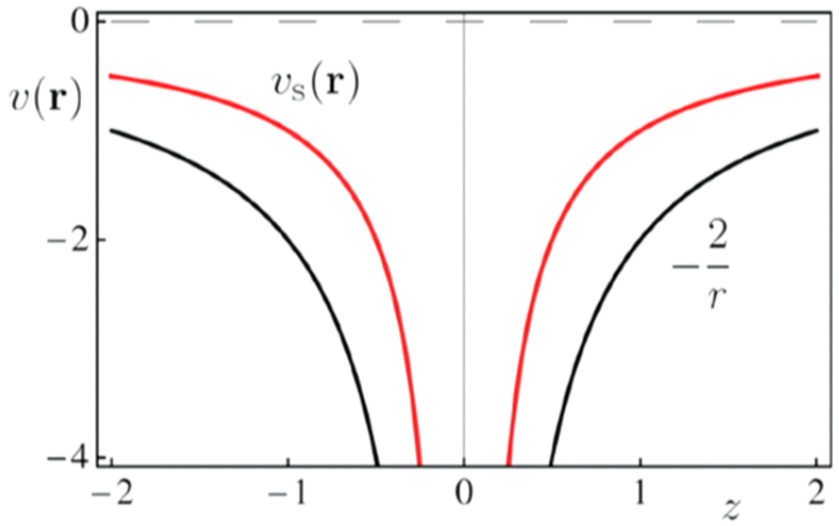
$$v_s^{(i)}(\vec{r}) \longrightarrow \underline{\Phi}^{(i)} \longrightarrow n^{(i)}(\vec{r})$$

2. Update $v_s^{(i+1)}(\vec{r}) = v(\vec{r}) + v_{HXC}[n^{(i)}](\vec{r})$

∞. Obtain g.s. energy $E[n] = T_s[n] + E_{HXC}[n] + \int v(\vec{r})\, n(\vec{r})$

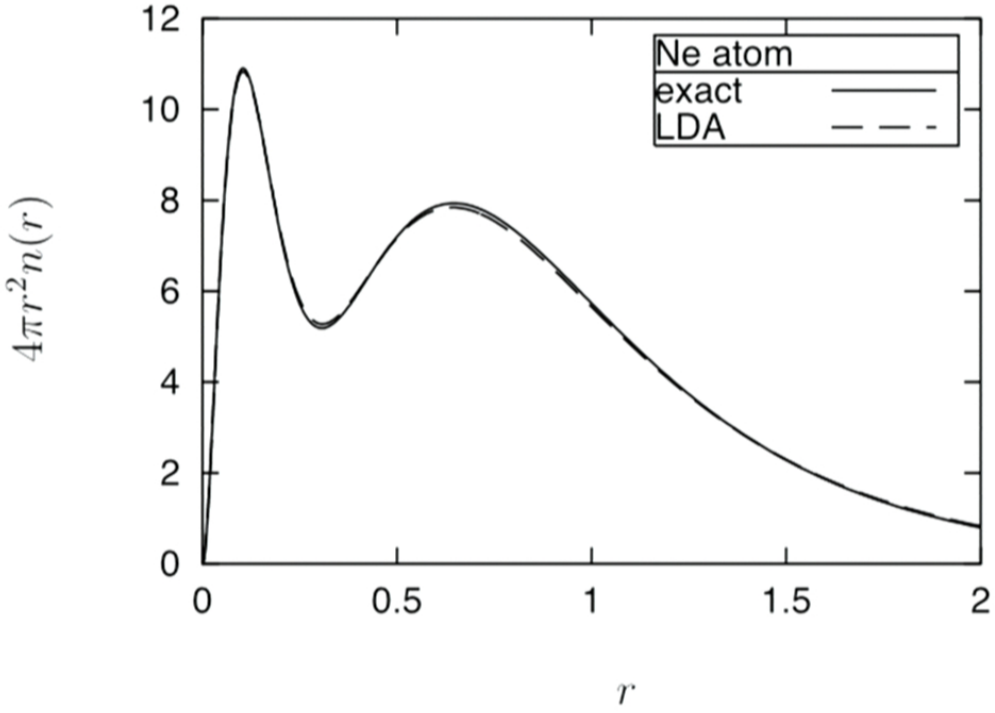
($\underline{\Phi}$) (LDA)

Exact Kohn-Sham potential of helium atom



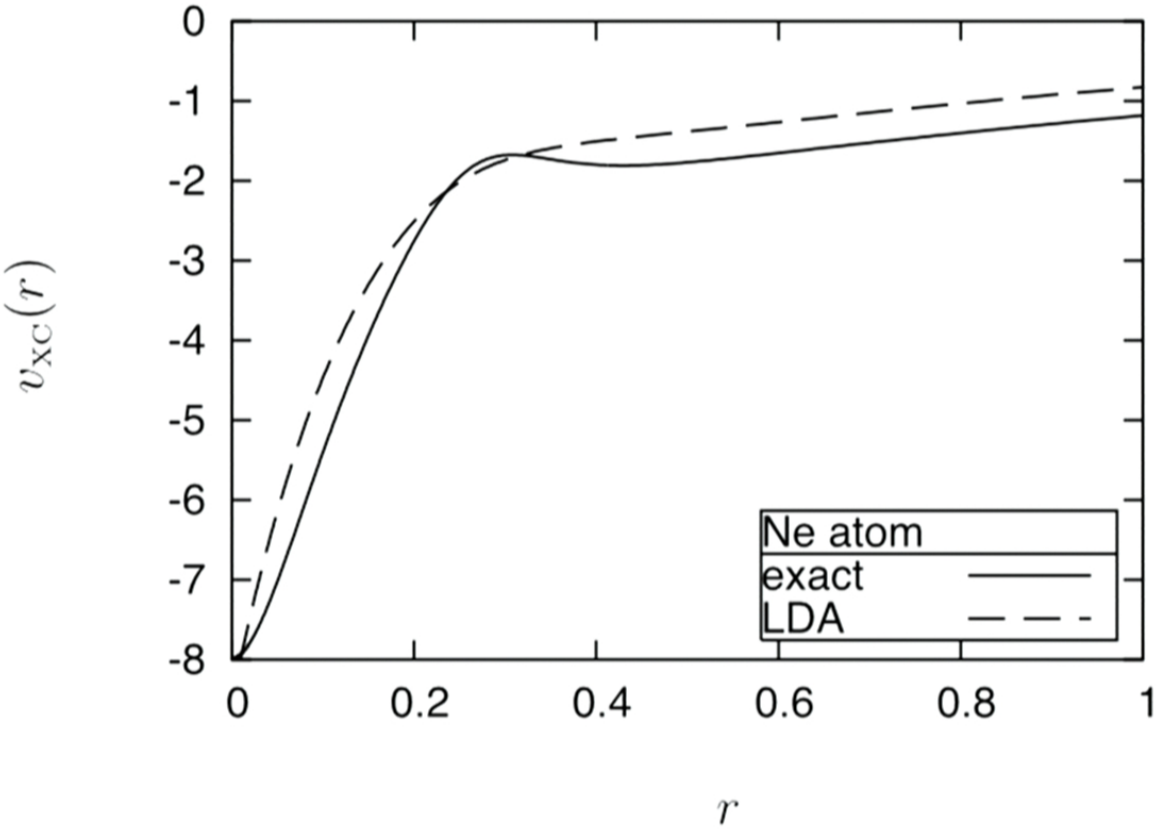
Umrigar and Gonze (1994)

Radial density of Ne atom, exact versus LDA



K. Burke "ABC of DFT"

Exchange-correlation potential of Ne atom, exact versus LDA



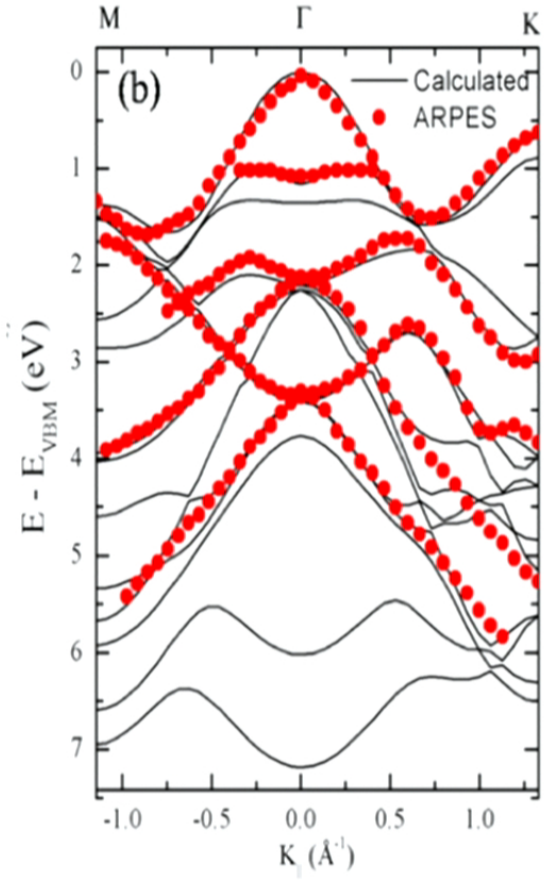
K. Burke "ABC of DFT"

Exact energy components of atoms

atom	E	T	V_{ext}	V_{ee}	T_{S}	U	E_{X}	T_{C}	U_{C}	E_{C}
He	-2.904	2.904	-6.753	0.946	2.867	2.049	-1.025	0.037	-0.079	-0.042
Be	-14.667	14.667	-33.710	4.375	14.594	7.218	-2.674	0.073	-0.169	-0.096
Ne	-128.94	128.94	-311.12	53.24	128.61	66.05	-12.09	0.33	-0.72	-0.39

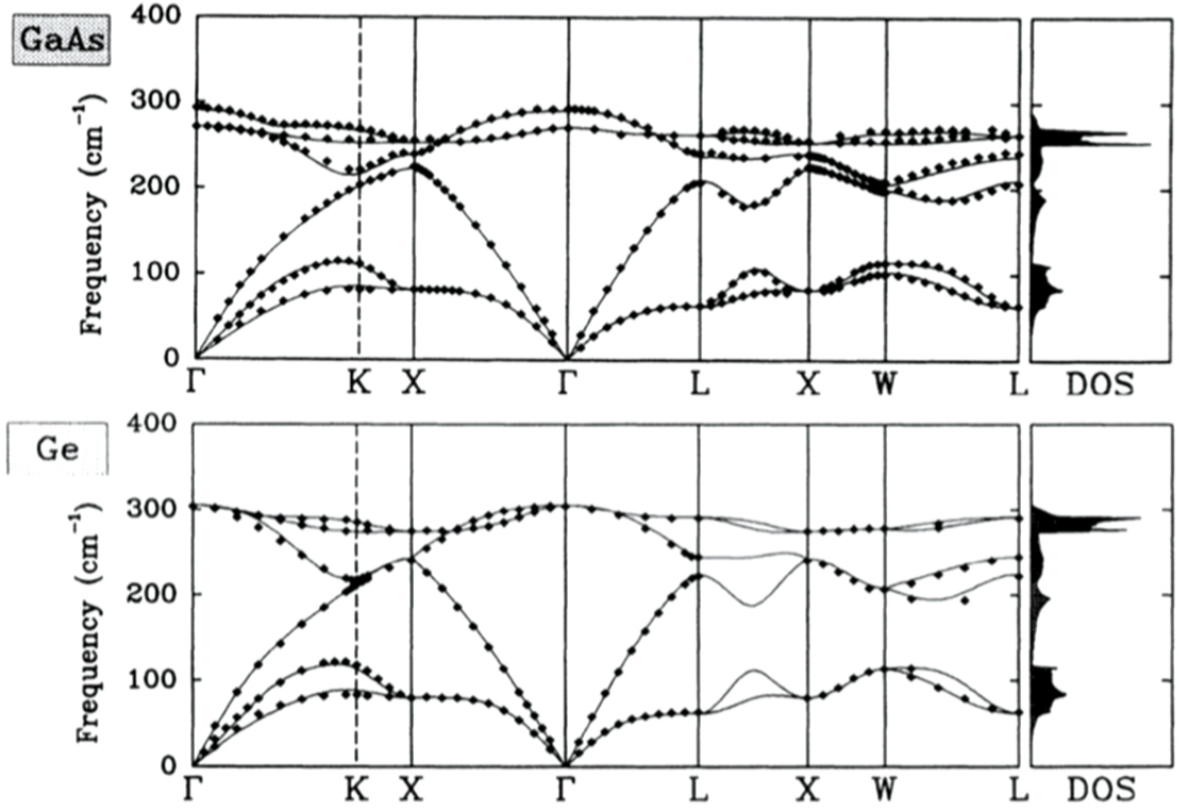
K. Burke "ABC of DFT"

DFT band structure of MoS_2 versus ARPES experiment

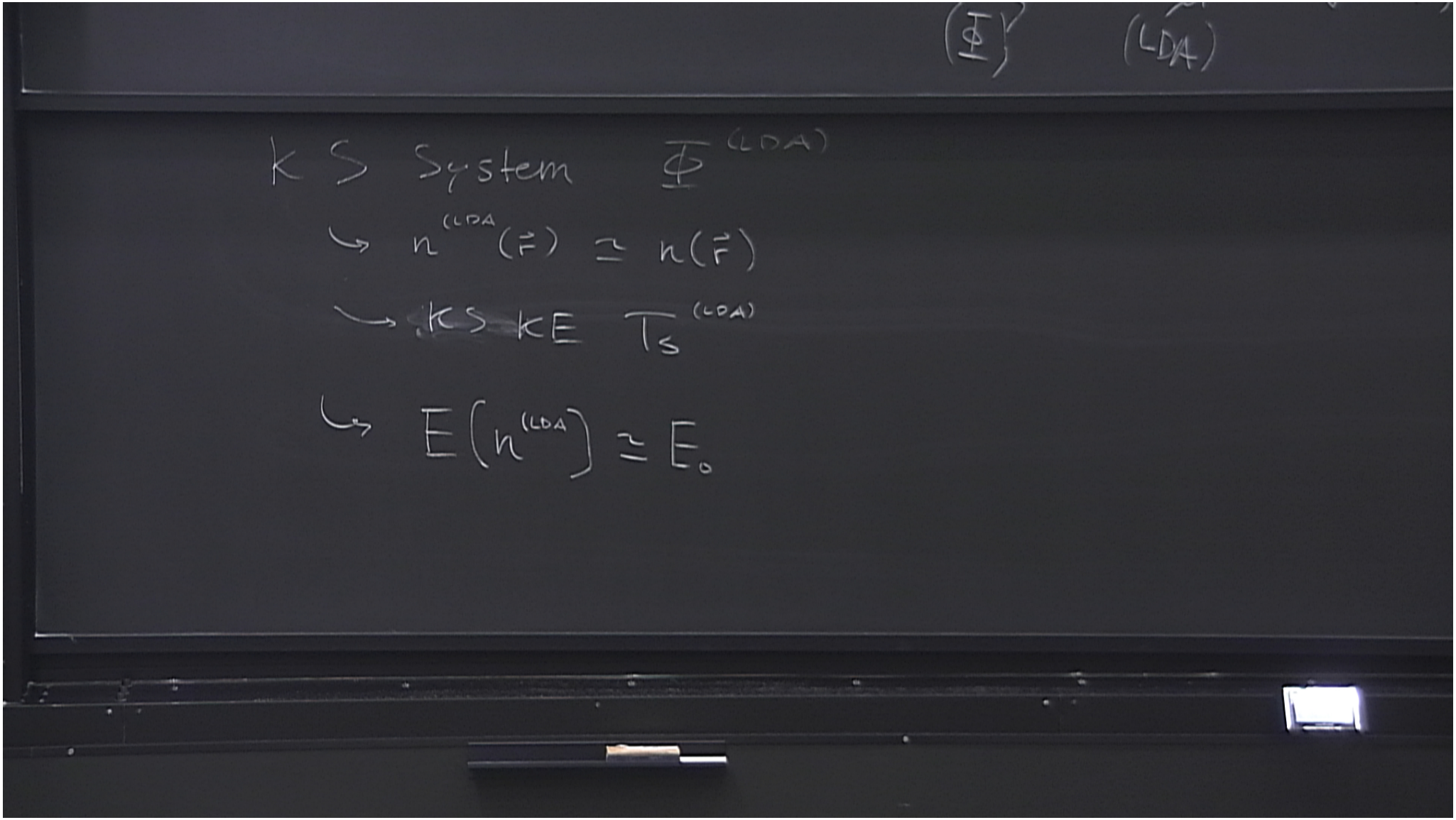


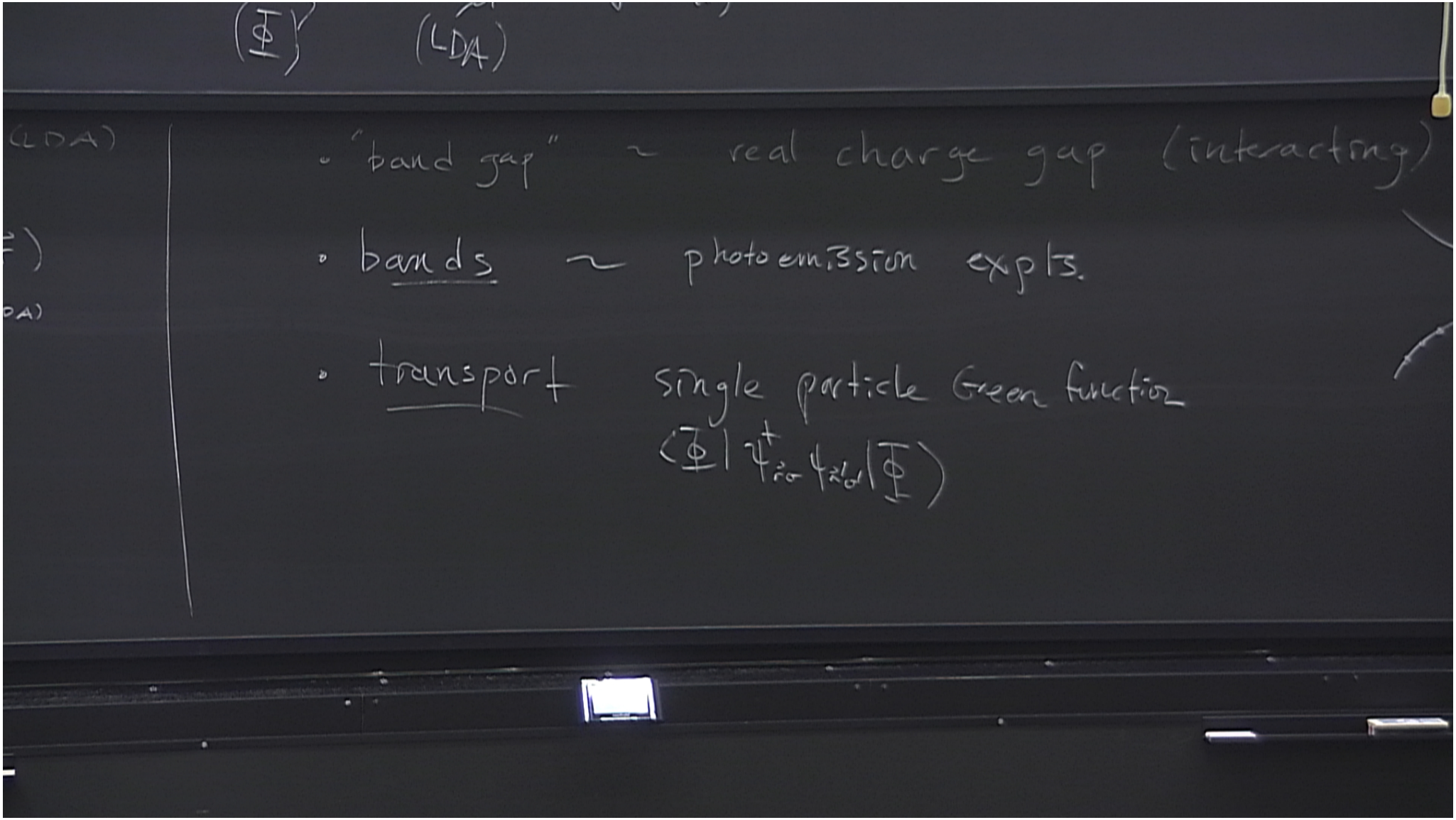
Mahatha et al., J. Phys. Cond. Mat. (2012)

Phonon spectra of GaAs and Ge computed from DFT, comparison to experimental data

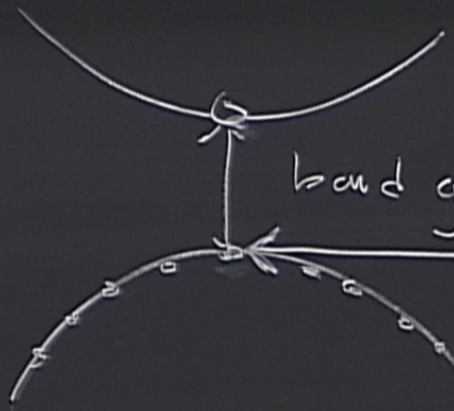


Giannozzi et al., PRB 43, 7231 (1991)


Φ (LDA)
KS System $\Phi^{(LDA)}$
$\hookrightarrow n^{(LDA}(\vec{r}) \simeq n(\vec{r})$
$\hookrightarrow$ KS KE $T_s^{(LDA)}$
$\hookrightarrow E(n^{(LDA}) \simeq E_0$

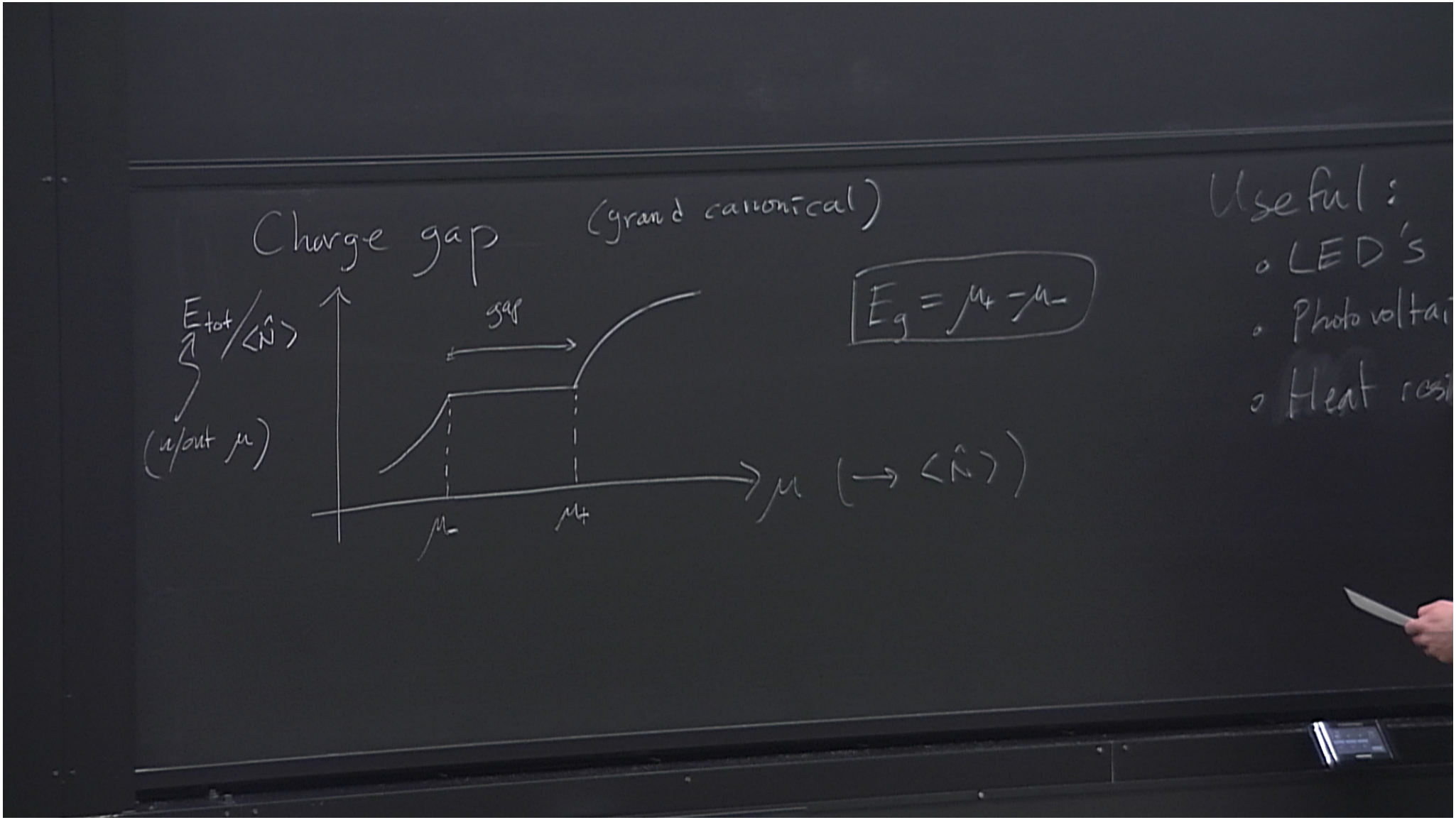

(LDA)
• "band gap" ~ real charge gap (interacting)
• bands ~ photoemission expts.
• transport single particle Green function

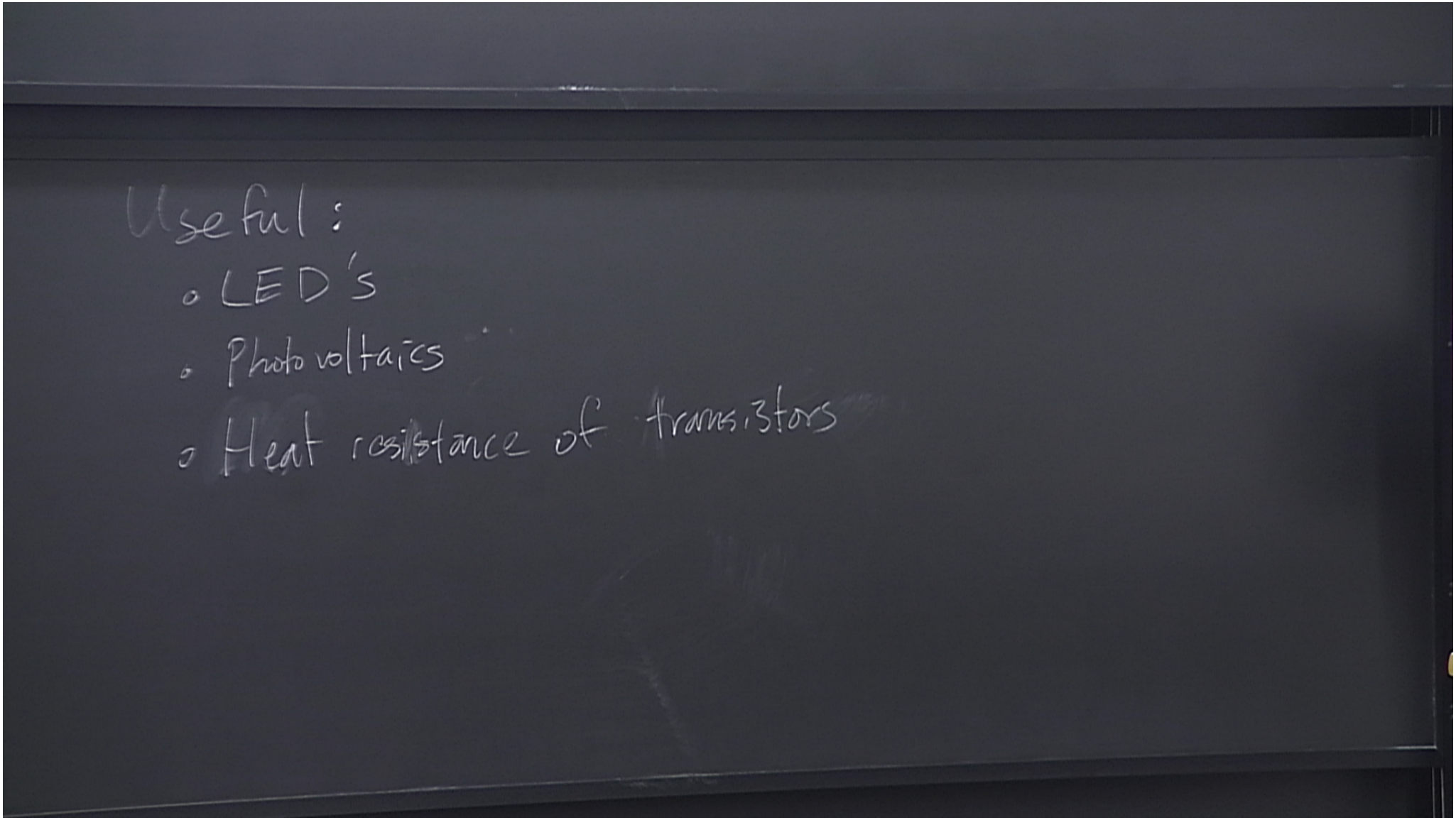
(interacting)

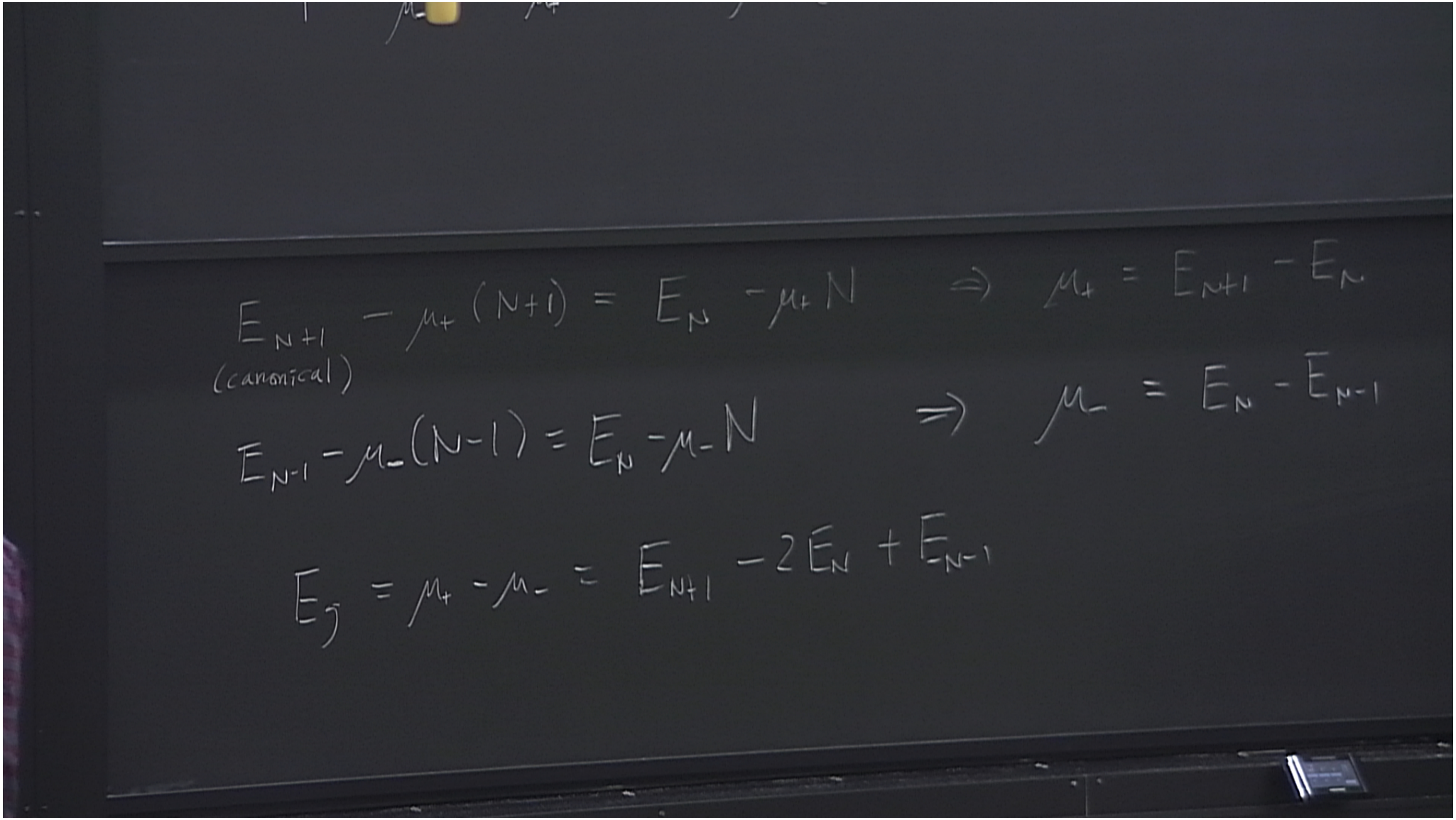


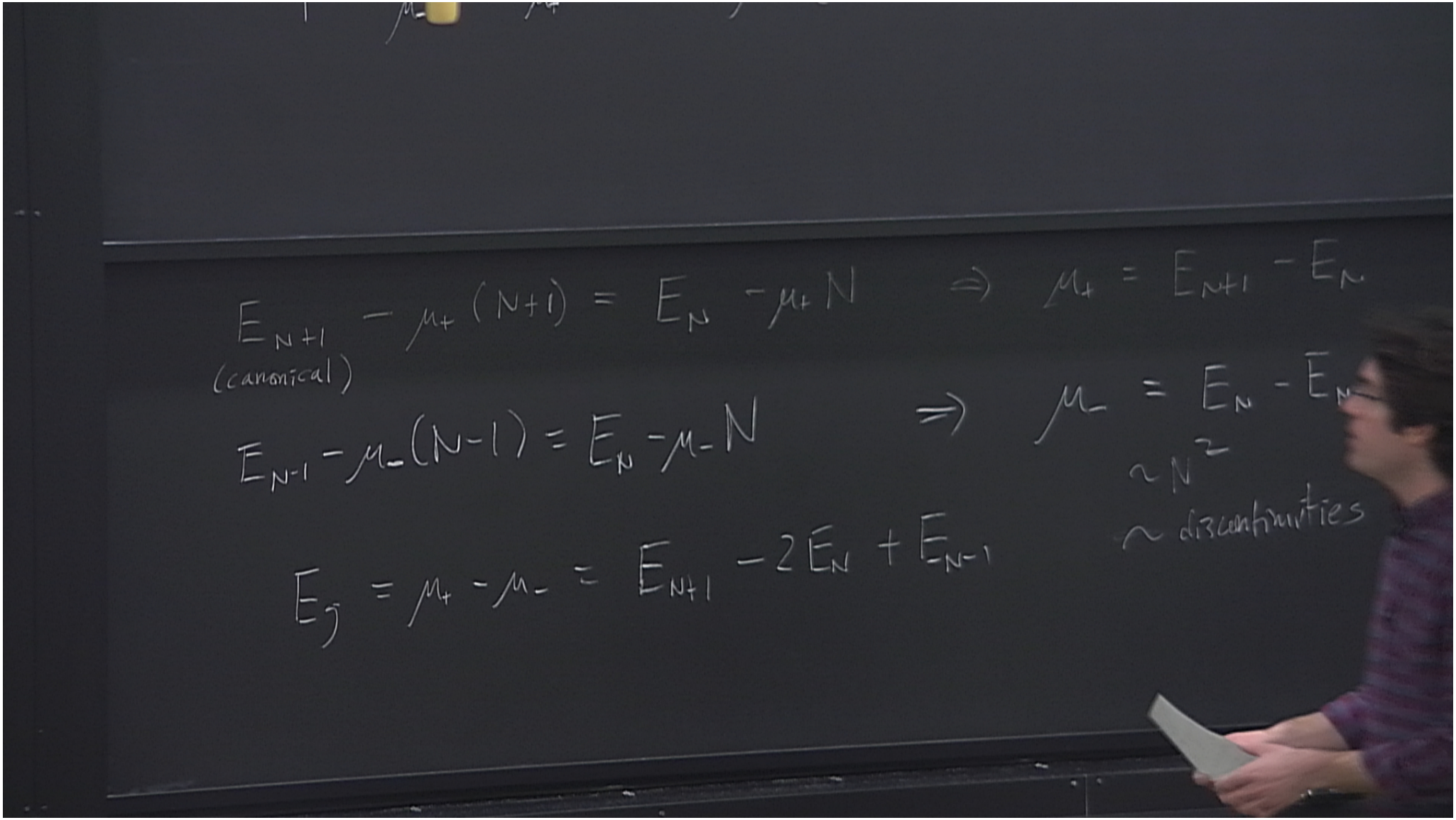
equals real value

(Koopmans' theorem)


Charge gap (grand canonical)
$E_{tot}/\langle\hat{N}\rangle$
(w/out μ)
gap
μ_-
μ_+
μ ($\rightarrow \langle\hat{N}\rangle$)
$E_g = \mu_+ - \mu_-$
Useful:
• LED's
• Photovolta
• Heat resi


Useful:
- LED's
- Photovoltaics
- Heat resistance of transistors


$E_{N+1} - \mu_+(N+1) = E_N - \mu_+ N \Rightarrow \mu_+ = E_{N+1} - E_N$
(canonical)
$E_{N-1} - \mu_-(N-1) = E_N - \mu_- N \Rightarrow \mu_- = E_N - E_{N-1}$
$E_g = \mu_+ - \mu_- = E_{N+1} - 2E_N + E_{N-1}$


$E_{N+1} - \mu_+ (N+1) = E_N - \mu_+ N \Rightarrow \mu_+ = E_{N+1} - E_N$
(canonical)
$E_{N-1} - \mu_- (N-1) = E_N - \mu_- N \Rightarrow \mu_- = E_N - E_N$
$\sim N^2$
$\sim$ discontinuities
$E_g = \mu_+ - \mu_- = E_{N+1} - 2E_N + E_{N-1}$

$v_s(\vec{r}) = v(\vec{r}) + v_{Hxc}[n^{(0)}](\vec{r})$

- Obtain g.s. energy $E[n] = T_s[n] + E_{Hxc}[n] + \int v(r)\, n(r)$

(Φ) (LDA)