Electronic-Structure Calculations in a 1D World

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Outline

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The local-density approximation (LDA)

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- Find the correlation energy of the **infinite** uniform electron gas (UEG) for all densities ρ
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☺ The LDA is an *ab initio* model with no adjustable parameters

☺ This is an attractive approach to molecular electronic structure

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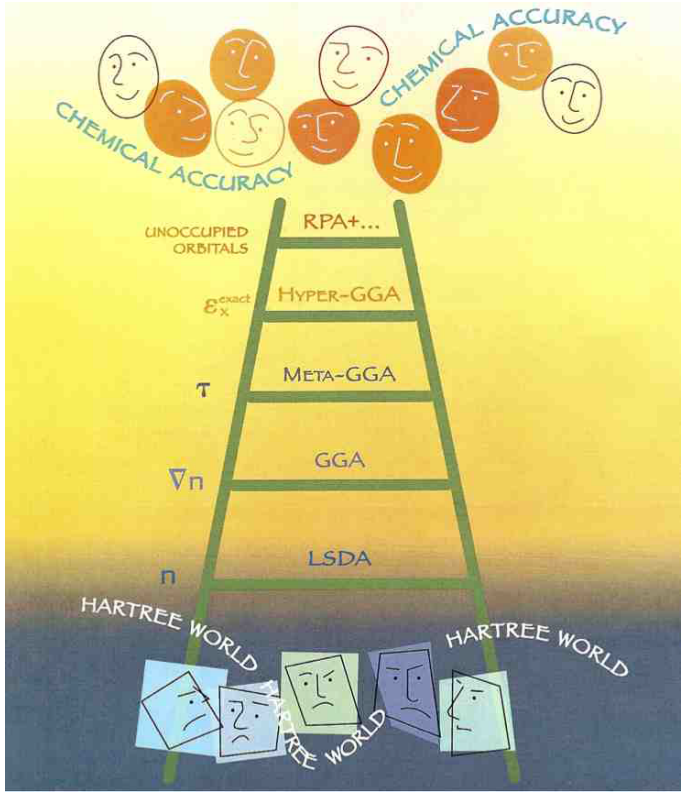
☹☹ Not very accurate for correlation energy (overestimated by roughly 100%)

Jacob's ladder vs Generalized LDA idea

- The lowest rung (LDA) assumes that all UEGs of density ρ are equivalent



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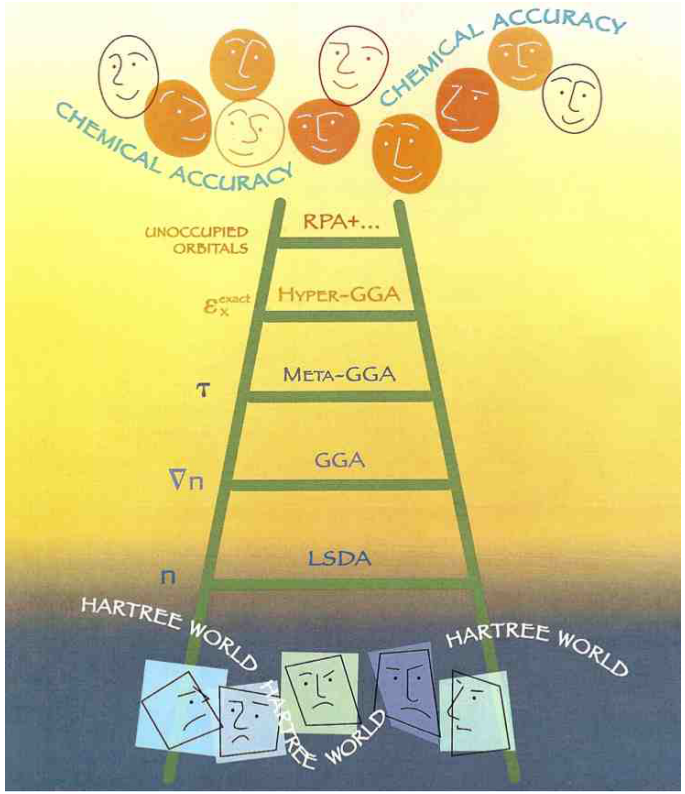

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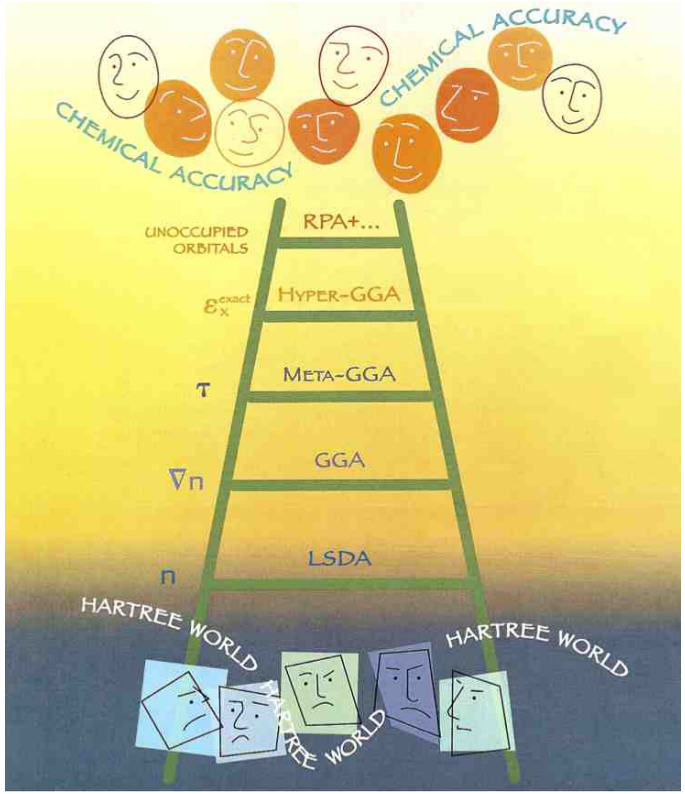

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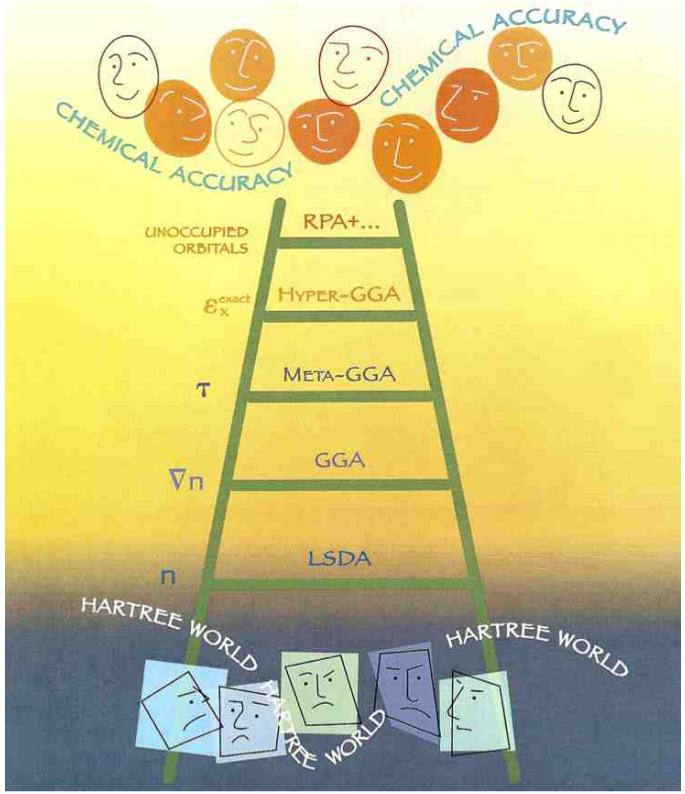
- We propose to follow an alternative route to heaven using finite-size UEGs!
- We add a new local two-electron parameter

$$\text{hole curvature: } \eta(\mathbf{r}) \propto 2\sum_{i}^{\text{occ}} |\nabla\psi_i|^2 - \frac{|\nabla\rho|^2}{2\rho}$$

Loos, Ball & Gill, J Chem Phys 140 (2014) 18A524



Finite-size UEGs in 1D Take 1: "Line" geometry

density: $\rho = \frac{1}{2\,r_s}$ and hole curvature: $\eta = 1 - \frac{1}{n^2}$

Reduced correlation energy (in millihartree) for n-electron system

		Seitz radius r_s										
n	η	0	0.1	0.2	0.5	1	2	5	10	20	50	100
2	3/4	14.168	13.914	13.679	13.011	12.032	10.463	7.563	5.236	3.303	1.619	0.894
3	8/9	19.373	18.962	18.581	17.526	16.031	13.739	9.735	6.662	4.170	2.030	1.119
4	15/16	21.917	21.404	20.939	19.657	17.873	15.205	10.671	7.265	4.531	2.199	1.210
5	24/25	23.373	22.804	22.272	20.845	18.886	15.997	11.166	7.579	4.717	2.286	1.257
6	35/36	24.293	23.672	23.109	21.582	19.508	16.477	11.462	7.765	4.827	2.336	1.284
7	48/49	24.916	24.270	23.669	22.075	19.919	16.792	11.654	7.885	4.897	2.369	1.301
8	63/64	25.361	24.686	24.070	22.421	20.208	17.011	11.786	7.967	4.945	2.391	1.313
9	80/81	25.691	24.996	24.363	22.676	20.418	17.170	11.881	8.026	4.979	2.407	1.321
10	99/100	25.943	25.229	24.588	22.870	20.577	17.289	11.952	8.070	5.005	2.416	1.328
∞	1	27.416	26.597	25.91	23.962	21.444	17.922	12.318	8.292	5.133	2.476	1.358

Lee & Drummond, Phys Rev B 83 (2011) 245114; Loos, Phys Rev A 89 (2014) 05252

Finite-size UEGs in 1D Take 2: "Ring" geometry

density: $\rho = \dfrac{1}{2\,r_s}$ and hole curvature: $\eta = 1 - \dfrac{1}{n^2}$

Reduced correlation energy (in millihartree) for n-electron system

		Seitz radius r_s										
n	η	0	0.1	0.2	0.5	1	2	5	10	20	50	100
2	3/4	13.212	12.985	12.766	12.152	11.250	9.802	7.111	4.938	3.122	1.533	0.848
3	8/9	18.484	18.107	17.747	16.755	15.346	13.179	9.369	6.427	4.030	1.965	1.083
4	15/16	21.174	20.698	20.249	19.027	17.324	14.762	10.390	7.085	4.425	2.150	1.184
5	24/25	22.756	22.213	21.66	20.33	18.439	15.644	10.946	7.439	4.636	2.248	1.237
6	35/36	23.775	23.184	22.63	21.14	19.137	16.192	11.285	7.653	4.762	2.307	1.268
7	48/49	24.476	23.850	23.24	21.70	19.607	16.554	11.509	7.795	4.844	2.345	1.289
8	63/64	24.981	24.328	23.69	22.11	19.940	16.808	11.664	7.890	4.901	2.370	1.302
9	80/81	25.360	24.686	24.04	22.39	20.186	16.995	11.777	7.960	4.941	2.389	1.312
10	99/100	25.651	24.960	24.25	22.62	20.373	17.134	11.857	8.013	4.973	2.404	1.320
∞	1	27.416	26.597	25.91	23.962	21.444	17.922	12.318	8.292	5.133	2.476	1.358

Loos & Gill, J Chem Phys 138 (2013) 164124; Loos, Ball & Gill, ibid 140 (2014) 18A524

GLDA correlation functional for 1D systems

$$E_c^{\mathrm{GLDA}}(r_s,\eta) = \Upsilon_0(\eta)\, F\left[1, \frac{3}{2}, \Upsilon(\eta), \frac{\Upsilon_0(\eta)(1-\Upsilon(\eta))}{\Upsilon_\infty(\eta)}\, r_s\right]$$

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$F(a,b,c,r_s)$	$=$	Hypergeometric function	$\Leftrightarrow$	exact for small and large r_s
$\Upsilon_0(\eta)$	$=$	electrons are close to each other	$\Leftrightarrow$	perturbation theory
$\Upsilon(\eta)$	$=$	intermediate densities	$\Leftrightarrow$	quantum Monte Carlo
$\Upsilon_\infty(\eta)$	$=$	electrons are far apart	$\Leftrightarrow$	perturbation theory

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By construction, $E_c^{\mathrm{GLDA}}(r_s,\eta=1) = E_c^{\mathrm{LDA}}(r_s)$ and $E_c^{\mathrm{GLDA}}(r_s,\eta=0) = 0$

Loos, Phys Rev A 89 (2014) 052523

Results for strongly- and weakly-correlated systems

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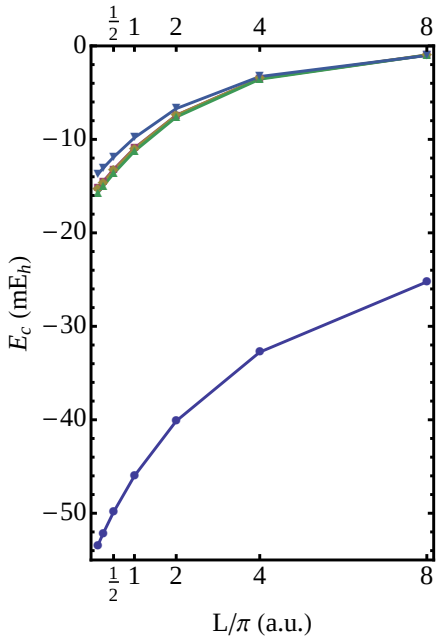
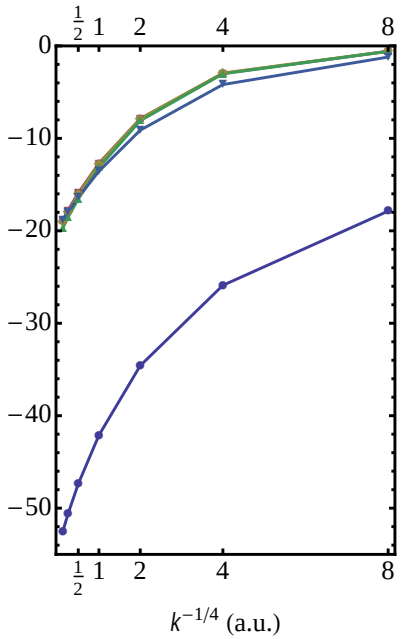




	Electrons in a box ($L = \pi$)					Electrons in a harmonic well ($k = 1$)				
	$n = 2$	$n = 3$	$n = 4$	$n = 5$	$n = 6$	$n = 2$	$n = 3$	$n = 4$	$n = 5$	$n = 6$
LDA	46	73	99	126	154	42	66	90	115	139
GLDA	11	27	45	65	86	13	29	46	65	84
FCI	10	26	46	68	92	14	32	52	74	101

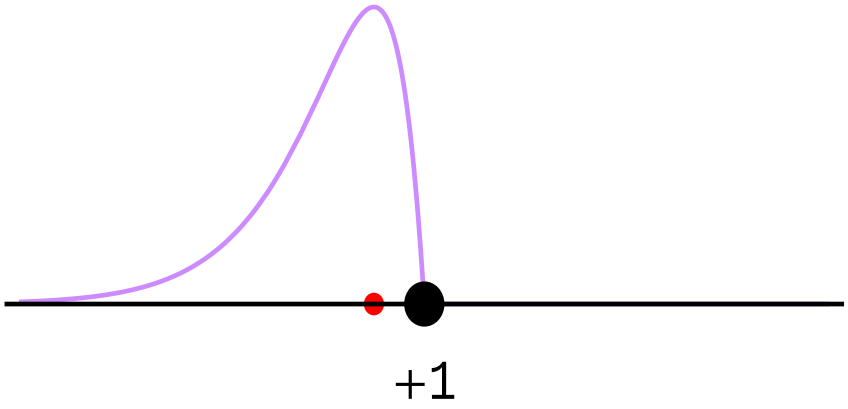
Outline

Impenetrability of the Coulomb potential $|x|^{-1}$ in 1D: H atom

Newton, J Phys A 27 (1994) 4717; Nunez-Yepez et al., Phys Rev A 83 (2011) 064101.

Hydrogen atom in 1D

Left-handed ground state: $_1$**H**



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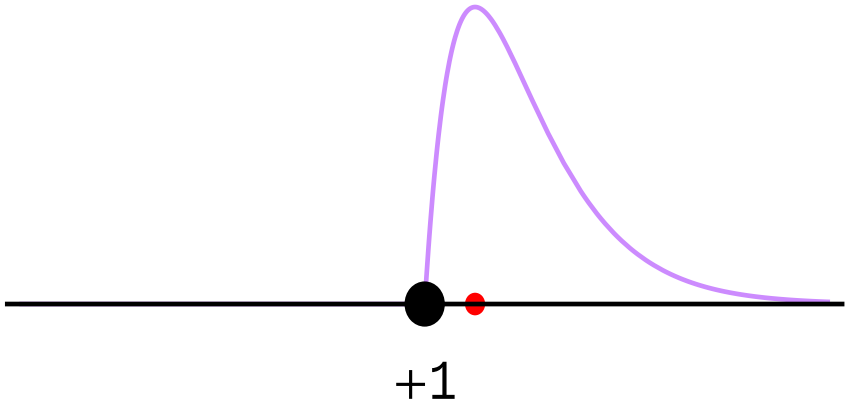

Loudon, Am J Phys 27 (1959) 649; Nunez-Yepez et al., Phys Rev A 83 (2011) 064101.

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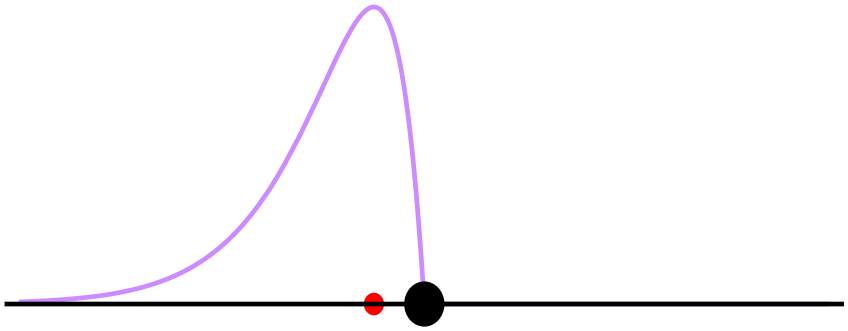

$$\boxed{\psi(x) = -x\exp(+x)}$$

$$E = -0.5$$

$$\mu = +1.5 \qquad R = \sqrt{\langle x^2 \rangle} = 1.8$$

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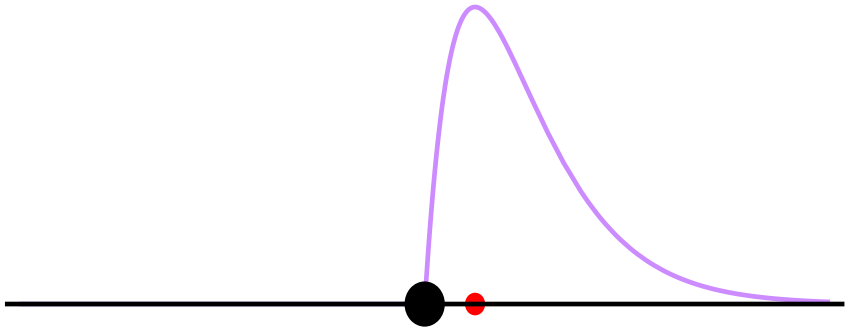

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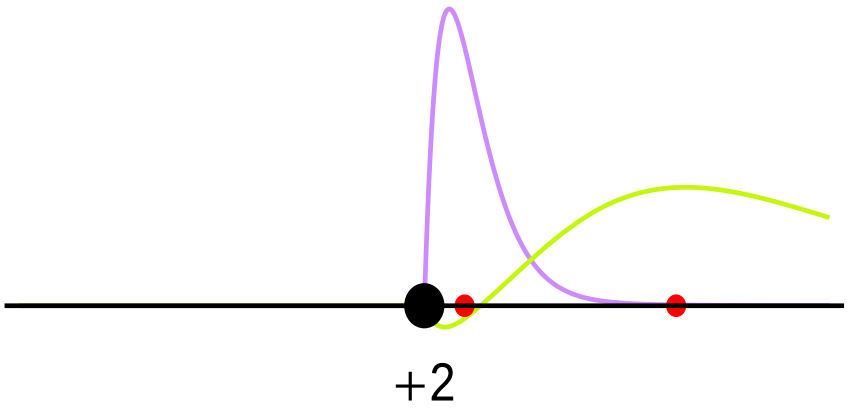
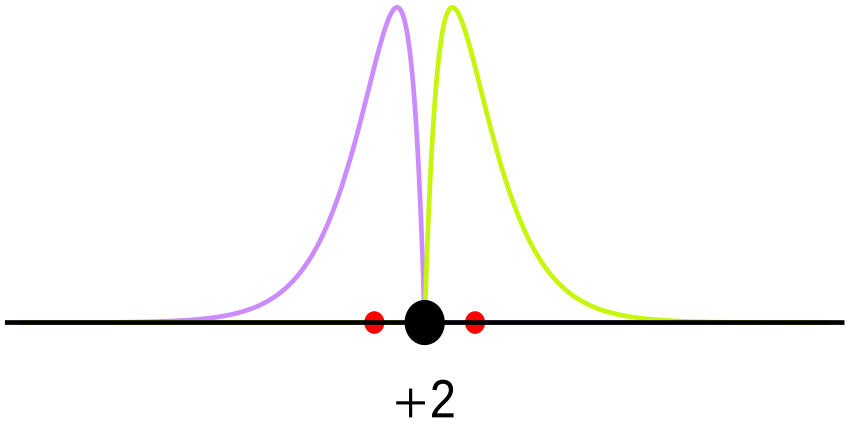
Helium atom in 1D

One-sided helium: $He_{1,2}$



Two-sided helium: $_1He_1$



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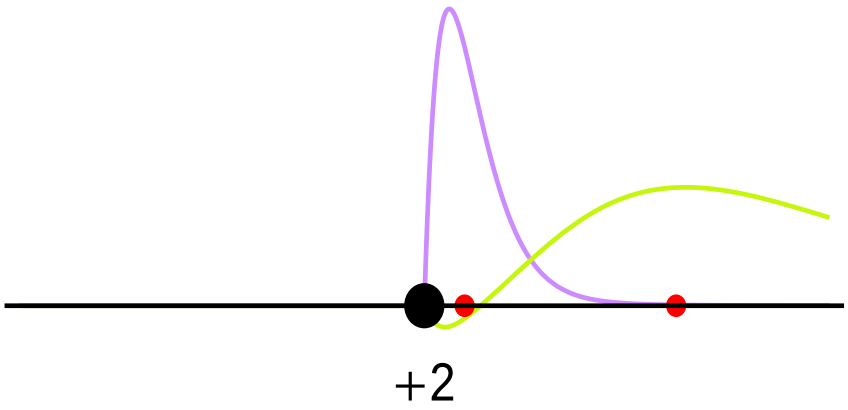

$E = -2.1074$

$\mu = +3.5 \qquad R = 4.8$

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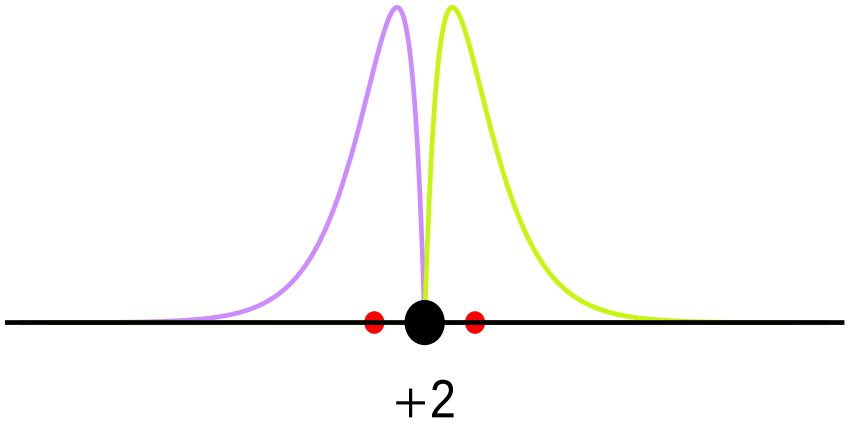
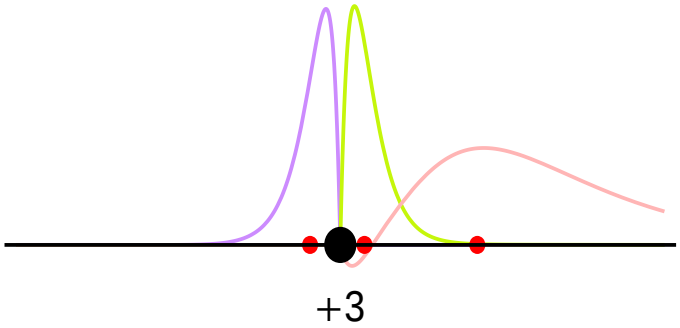


$E = -3.2429$

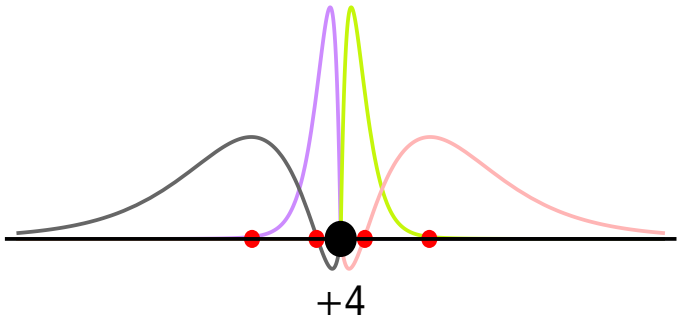
$\mu = 0 \qquad R = 1.0$

More 1D atoms...

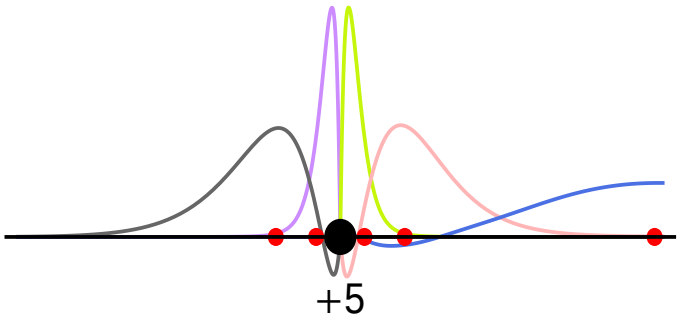
Lithium: $\mu = 1.5$ **and** $R = 2.8$



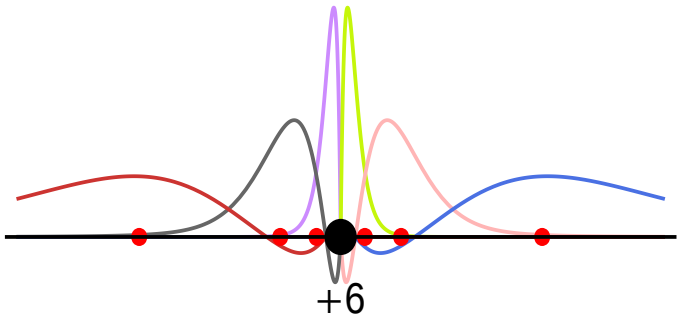
Beryllium: $\mu = 0$ **and** $R = 2.1$



Boron: $\mu = 1.9$ **and** $R = 4.7$



Carbon: $\mu = 0$ **and** $R = 3.7$



The periodic table in a 1D world...

Periodic trends in 1D atoms

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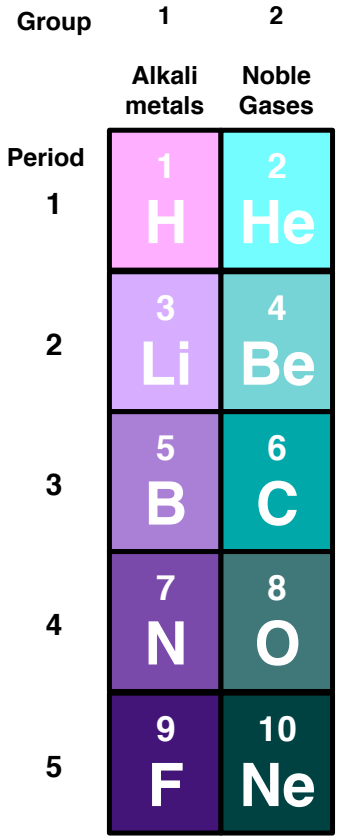

How good is GLDA for 1D atoms?

	Negative correlation energies (mEh)				
	LDA	GLDA	MP2	MP3	Exact
H_1	19	0	0	0	0
$_1He_1$	43	0	2	3	3
$_1Li_{1,2}$	61	3	3	4	4
$_{1,2}Be_{1,2}$	84	10	7	8	—
$_{1,2}B_{1-3}$	102	16	10	11	—
$_{1-3}C_{1-3}$	123	24	15	17	—
$_{1-3}N_{1-4}$	140	31	19	22	—
$_{1-4}O_{1-4}$	161	39	25	28	—
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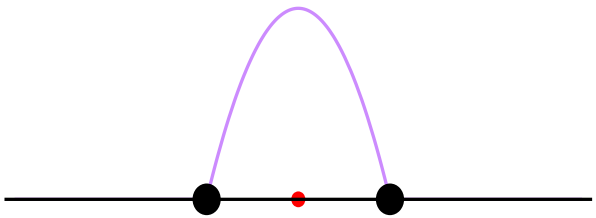
- ☹ GLDA is missing the dispersion-type correlation energy!
- ☺ Easy to fix...

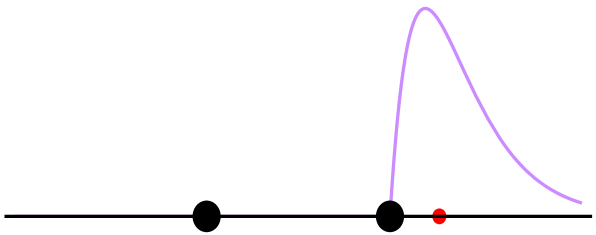
Outline

The H_2^+ molecule in 1D

The H_1H^+ state: $\mu = 0$



The $HH_1{}^+$ state: $\mu \neq 0$



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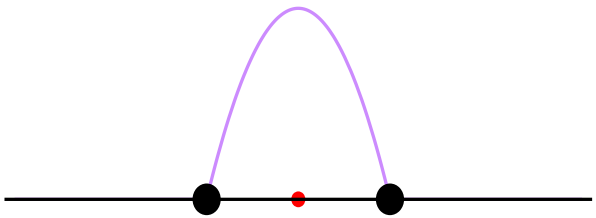

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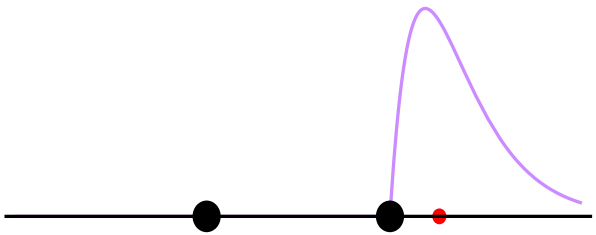
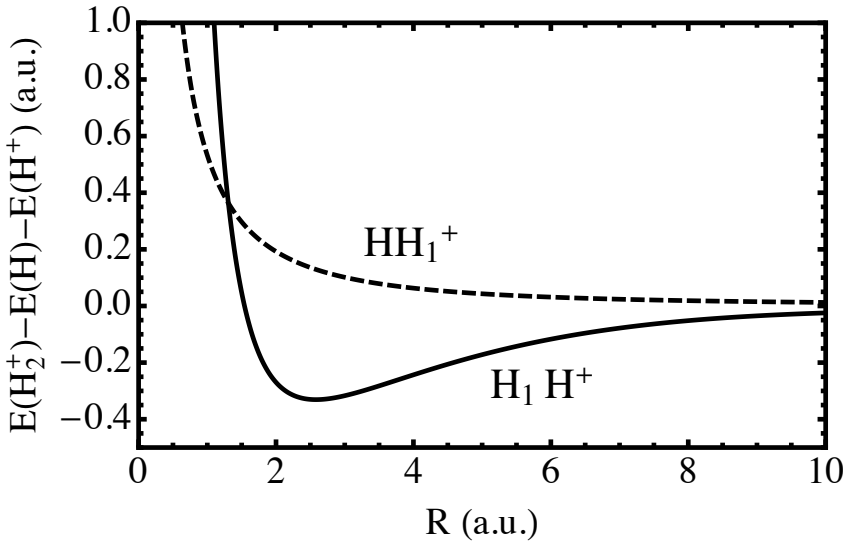
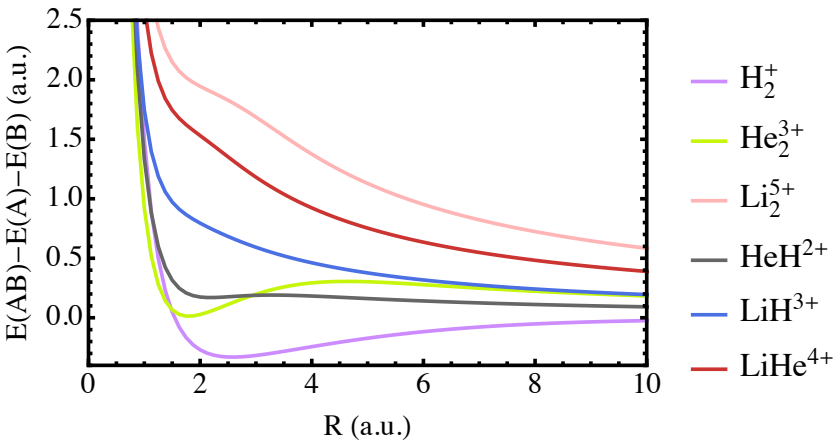


Potential energy curves for H_2^+

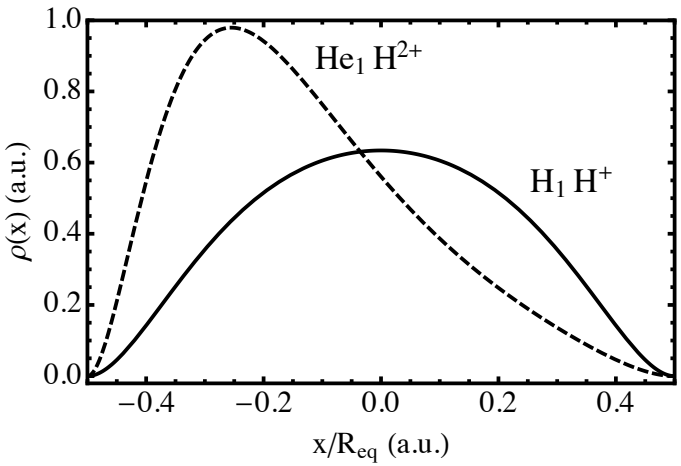


One-electron diatomic molecules in 1D

Potential energy curves for H_2^+-like molecules

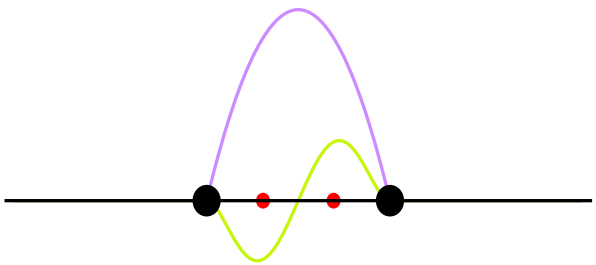


Electron densities for one-electron diatomics

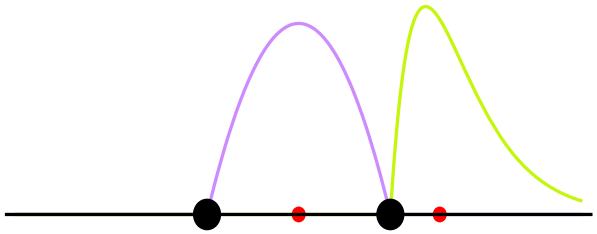


The H_2 molecule in 1D

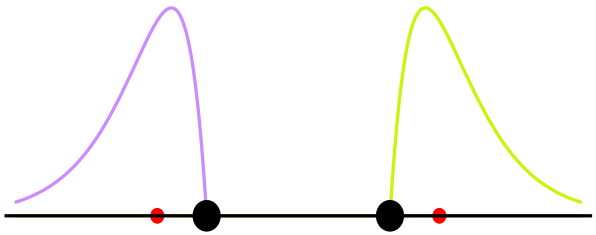
The $H_{1,2}H$ state



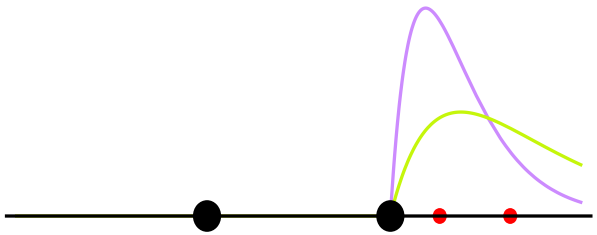
The H_1H_1 state



The $_1HH_1$ state

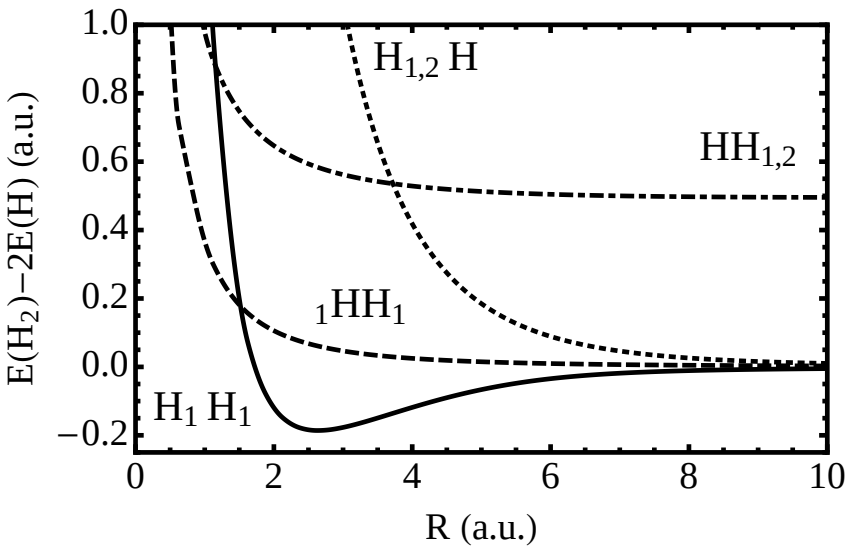


The $HH_{1,2}$ state

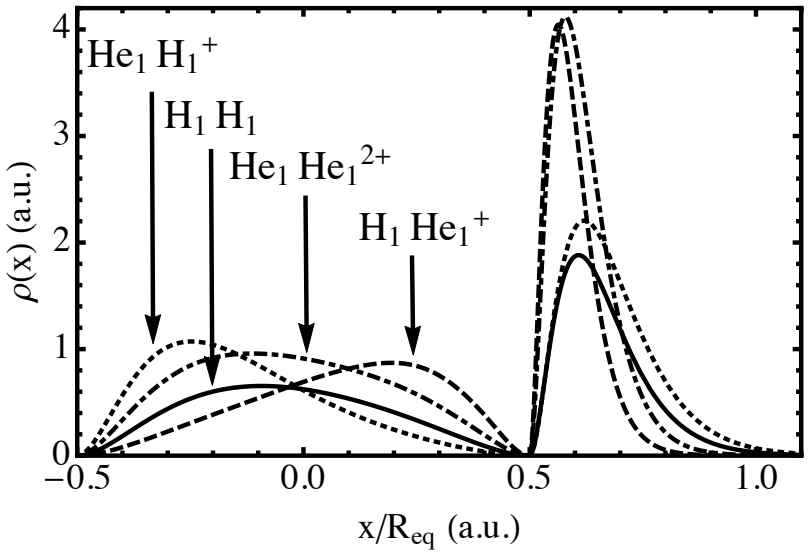


Two-electron diatomic molecules in 1D

Potential energy curves for the H_2 molecule



Electron densities for two-electron diatomics



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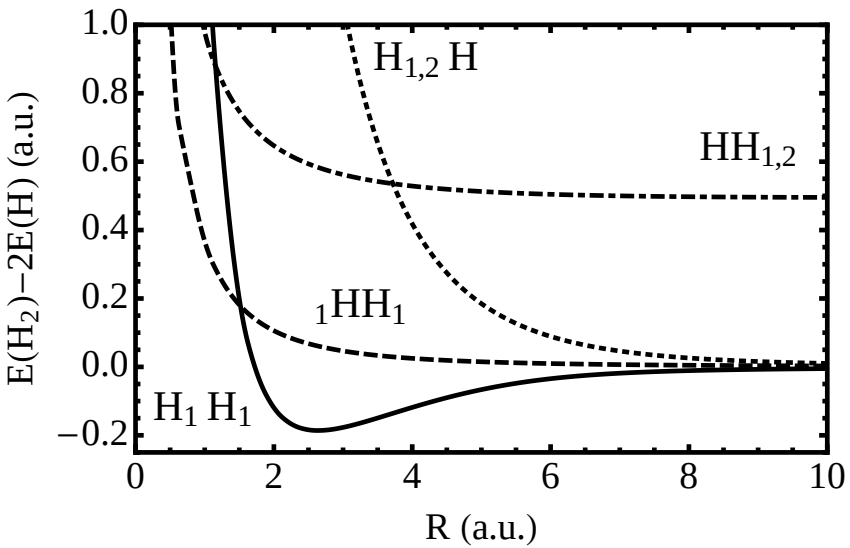

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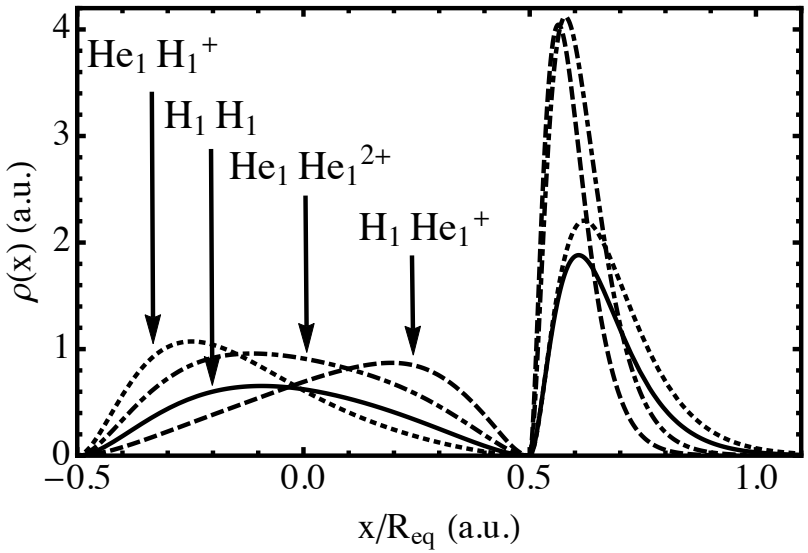
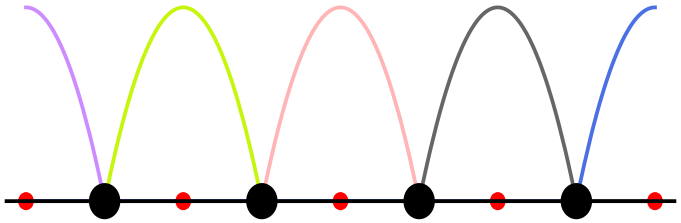


1D atoms are bound by one-electron bonds!!

Lego-style formation of 1D polymers



- A single H_1 atom has a dipole moment

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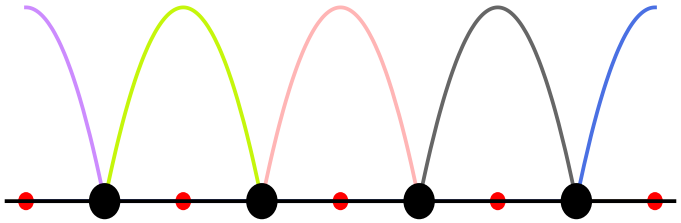

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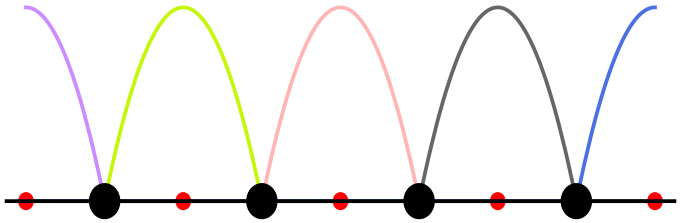

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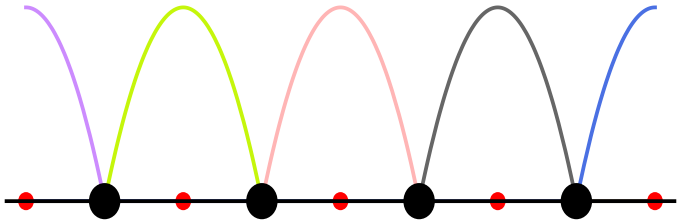

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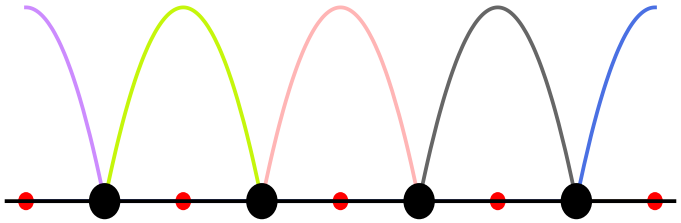

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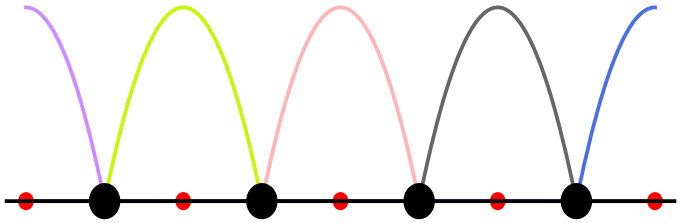

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Take-home messages

- All uniform electron gases are equal, but some are more equal than others!
- GLDA improves LDA (a lot)
- 1D chemistry is very different from 3D chemistry
- Electrons cannot penetrate the nuclei
- Periodic Table has only two groups: alkali metals and noble gases
- Dipole-dipole contribution to bonding is important
- 1D atoms are bound by one-electron bonds!