

TABLE II: Various components of the total energy of the helium atom. Results are reported for single-particle wave functions and eigenenergies coming from self-consistent LSDA or Hartree-Fock (HF) calculations. Energies are in Hartree. Except for the (\*) values, all calculations use a radial grid of size  $r_{max} = 18$  Bohr radii and  $N_{max} = 257$  single-particle states for each angular momentum channel. The starred (\*) values are difficult to converge, and the values in the table are uncertain to within  $\pm 0.001$ : see text for details. For reference, the exact (CI) non-relativistic correlation energy is also shown as the last entry.

Energy component	Equation	LSDA	HF	Difference
Kinetic		2.768	2.862	1.0%
Electron-ion		-6.626	-6.749	1.0%
Hartree		1.996	2.052	1.0%
Fock exchange	(22)	-0.998	-1.026	1.0%
$\Phi_c$ : $W(0)$ instead of $W_t(0)$	(50)	-0.318	-0.255	25%
$\Phi_c$ : square root approx.	(49)	-0.311	-0.248	25%
$\Phi_c$ : static approx.	(46)	-0.313	-0.250	25%
$\Phi_c$ : main approx.	(45)	-0.060*	-0.048*	25%
$\Phi_c$ : RPA	(38)	-0.081	-0.064	27%
$\Phi_c$ : CI (exact) Ref. [67]		-0.0420		

timate the importance of correlations and give too negative values uniformly. We discuss the reason for this in the next paragraph, but in the meantime we see that once the static approximation is made, the various forms for the correlation energy are quite similar. For example, the difference between the square root form of Eq. (46) and its series expansion in Eq. (49) is small. The smallness of the differences simply means that the ratio  $\langle W(0) \rangle / \Delta$  is small: *e.g.*, for boron we find the largest value of the ratio  $\langle W(0) \rangle / \Delta$  is 0.2 and is achieved for the  $2s$ - $2p$  transition. Given how far all these static correlation energies are from the dynamic answer of Eq. (45) or the exact RPA answer of Eq. (38), one can take all these static approximations to be basically of equal accuracy.

The reason the static approximations overestimate the magnitude of the correlation energy is easy to understand. Figure 3 shows how three representative correlation energies converge for the case of atomic boron: the static formula of Eq. (46), the dynamic formula of Eq. (45), and the exact RPA formula of Eq. (38). What is shown is the correlation energy contributions summed up to a given transition energy (or plasmon energy for the exact case). In all cases, we see that the contributions to the correlations are small, then become large at a certain energy, and then become smaller again. In atomic boron at LSDA level, there are two physically important transitions: the dominant  $2s$ - $2p$  at 0.21 Ha and then the weaker