FIG. 3: Convergence of correlation energies for the boron atom. Both plots show the cumulative sum of the contributions to the correlation energies (vertical) for transitions and/or plasma modes up to some given energy Δ_t (horizontal). LSDA wave functions and eigenenergies are used with a radial grid of size $r_{max} = 40$ Bohr radii and $N_{max} = 400$ eigenstates. The lowest solid black curve is for the static approximation of Eq. (46), the middle red dashed curve is for the dynamic approximation of Eq. (45), and the uppermost green dotted curve is for the exact RPA formula of Eq. (38). The plots show the same data with the only difference being a linear (top plot) or a logarithmic scale (bottom plot) of the horizontal axis. The dominant transitions in LSDA boron are the $2s$–$2p$ at 0.21 Ha and $1s$-$2p$ at 6.4 Ha, both visible in the lower plot as energies where the correlation contributions have a sudden jump.

have the dynamic and static matrix elements

$$\langle t|W_t(\Delta_t)|t\rangle = \langle t|V|t\rangle + \sum_p \frac{2\tilde{\omega}_p|\langle t|V|\tilde{p}\rangle|^2}{\Delta_t^2 - \tilde{\omega}_p^2},$$

$$\langle t|W_t(0)|t\rangle = \langle t|V|t\rangle - \sum_p \frac{2\tilde{\omega}_p|\langle t|V|\tilde{p}\rangle|^2}{\tilde{\omega}_p^2}.$$

Clearly, the static formula always gives negative correlation contributions that become small