

Figure 6.1 Behavior of e^x where $x = r$ (solid line, STO) and $x = r^2$ (dashed line, GTO)

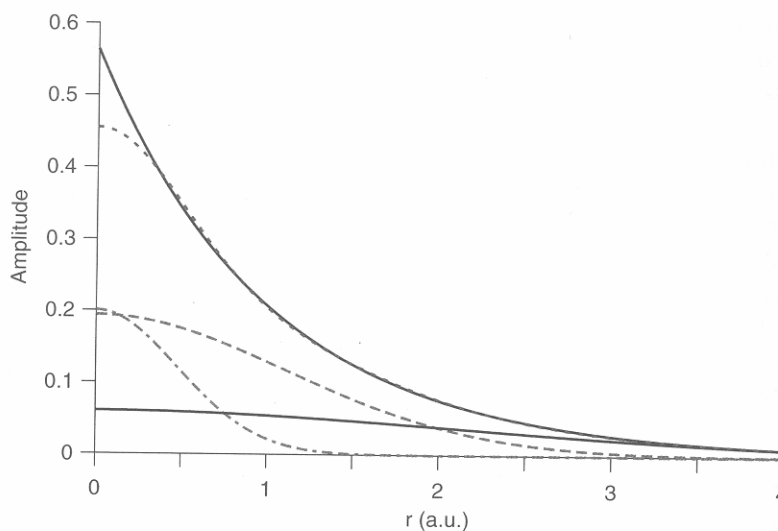


Figure 6.2 The radial behavior of various basis functions in atom-centered coordinates. The bold solid line at top is the STO ($\zeta = 1$) for the hydrogen 1s function; for the one-electron H system, it is also the exact solution of the Schrödinger equation. Nearest it is the contracted STO-3G 1s function (-----) optimized to match the STO. It is the sum of a set of one each tight (-----), medium (----), and loose (——) Gaussian functions shown below. The respective Gaussian primitive exponents α are 2.227660, 0.405771, and 0.109818, and the associated contraction coefficients c are 0.154329, 0.535328, and 0.444635. Note that from 0.5 to 4.0 a.u., the STO-3G orbital matches the correct orbital closely. However, near the origin there is a notable difference and, were the plot to extend to very large r , it would be apparent that the decay of the STO-3G orbital is more rapid than the correct orbital, in analogy to Figure 6.1

From Christopher J. Cramer, *Essentials of Computational Chemistry*
2nd Edition; Wiley: Chichester, England, 2004.