

## Solution to Exercise 4

a) With the given gaussians, the inner product  $\langle i|j\rangle$  is

$$\begin{aligned}\langle i|j\rangle &= C^2 \int dx e^{-\kappa(x-ia)^2 - \kappa(x-ja)^2} \\ &= C^2 \int dx e^{-\kappa(2x^2 - 2(i+j)ax + (i^2+j^2)a^2)} \\ &= C^2 e^{-\kappa a^2(i-j)^2/2} \int e^{-2\kappa(x-(i+j)a/2)^2} \\ &= C^2 e^{-\kappa a^2(i-j)^2/2} \cdot \sqrt{\pi/2\kappa}\end{aligned}$$

where we have completed the square in the exponent, as suggested in the exercise. In this exercise, all integrals extend from  $-\infty$  to  $+\infty$ . As long as  $\kappa a^2/2 \gg 1$ , and choosing  $C = (2\kappa/\pi)^{1/4}$ , we have

$$\langle i|j\rangle \simeq \delta_{ij}.$$

b) From the lectures, we have

$$\begin{aligned}\gamma &= -\langle 1| \sum_{m \neq 1} V_m |2\rangle \\ \varepsilon_0 &= \alpha - \alpha' = -\langle 2| \sum_{m \neq 2} V_m |2\rangle + \langle 1| \sum_{m \neq 1} V_m |1\rangle\end{aligned}$$

In the notation of the lectures (p 29), we have here chosen  $j = l = 1$  in the matrix element  $\alpha'$ ,  $j = l = 2$  in the matrix element  $\alpha$ , and  $j = l - 1 = 1$  in the matrix element  $\gamma$ . Each of these matrix elements is a sum over the index  $m$ , and all terms are, at the outset, assumed to be "small". The largest of these small terms correspond to  $m = 2$  in  $\gamma$ ,  $m = 2$  in  $\alpha'$ , and  $m = 1$  and  $m = 3$  in  $\alpha$ . All these terms in  $\alpha$  and  $\alpha'$  are equal. Hence, if we keep only the largest term(s) in the sums over  $m$ , we end up with

$$\begin{aligned}\gamma &= -\langle 1|V_2|2\rangle \\ \varepsilon_0 &= -\langle 1|V_2|1\rangle\end{aligned}$$

Here, both matrix elements are integrals of products of gaussians. Just like in a), we may solve the integral by completing the square in the exponent. This yields

$$\begin{aligned}\gamma/C^2V_0 &= \sqrt{\frac{\pi}{2\kappa + \beta}} \exp\left(-a^2 \cdot \frac{\kappa^2 + \kappa\beta}{2\kappa + \beta}\right) \\ \varepsilon_0/C^2V_0 &= \sqrt{\frac{\pi}{2\kappa + \beta}} \exp\left(-a^2 \cdot \frac{2\kappa\beta}{2\kappa + \beta}\right)\end{aligned}$$

and finally

$$y = \frac{\varepsilon_0}{\gamma} = \exp\left(a^2 \cdot \frac{\kappa(\kappa - \beta)}{2\kappa + \beta}\right),$$

which is larger than 1 if  $\kappa > \beta$ , i.e., if  $|j\rangle$  decays faster than  $V_j$ .