PC4902 Solutions: Addendum

At the end of question 1.1 you were asked to show *explicitly* that the ground-state energy of the Hubbard molecule was smaller than Hartree–Fock approximation to it:

Now, for any t and U,

$$\left(U - \sqrt{U^2 + 16t^2}\,\right)\left(U + \sqrt{U^2 + 16t^2}\,\right) = -16t^2,$$

so

$$\tfrac{1}{2}U - \tfrac{1}{2}\sqrt{U^2 + 16t^2} = \frac{-8t^2}{U + \sqrt{U^2 + 16t^2}}.$$

But the denominator on the right-hand side increases with t^2, reaching the value $4U$ when $t^2 = \frac{1}{2}U^2$. Hence

$$\tfrac{1}{2}U - \tfrac{1}{2}\sqrt{U^2 + 16t^2} < -8t^2/(4U) = -2t^2/U \quad \text{for } t < U/\sqrt{2}.$$

The right-hand side coincides the Hartree-Fock result for $t < \frac{1}{2}U$, which is within the range required by $t < U/\sqrt{2}\,$.

The inequality needed for $t > \frac{1}{2}U$ is much easier to establish. Indeed, for *any* $U \neq 0$ we have $U^2 + 16t^2 \geq 16t^2$, so

$$E_0 = -\tfrac{1}{2}\sqrt{U^2 + 16t^2} + \tfrac{1}{2}U < -\tfrac{1}{2}\sqrt{16t^2} + \tfrac{1}{2}U = -2t + \tfrac{1}{2}U,$$

which is the Hartree–Fock result for $t \geq \frac{1}{2}U$.