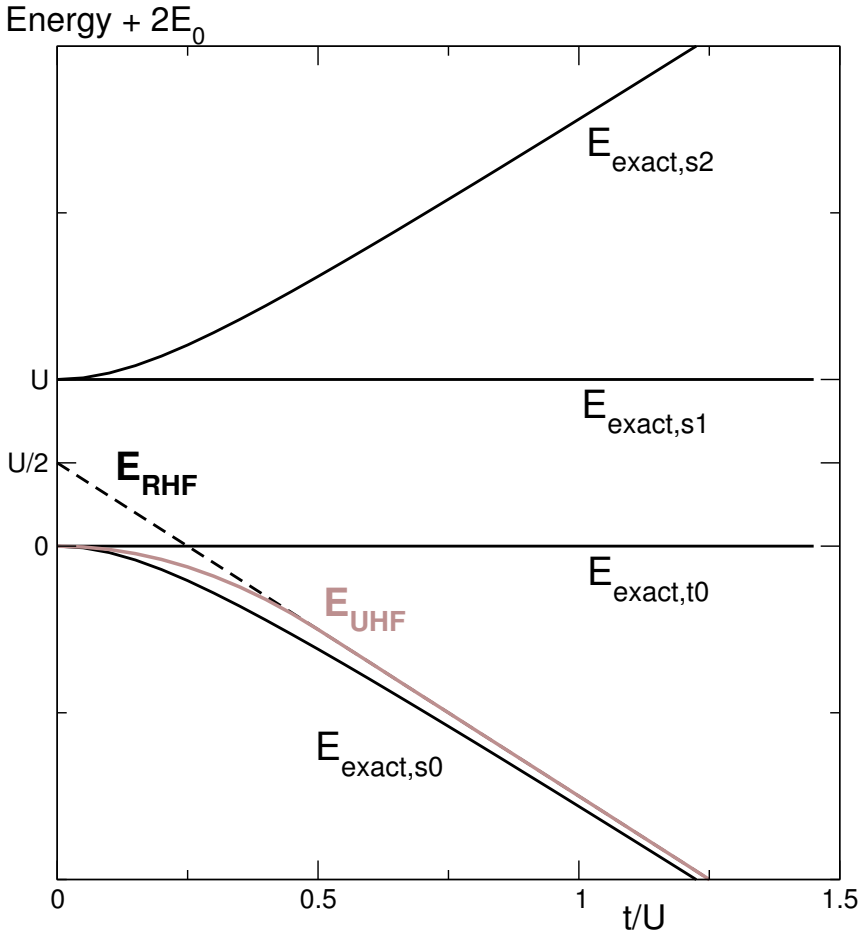
Correction

The figure shows the energy of different level in units of U (shifted by the quantity $2E_0$).



In the following we assume the 2-electron energies to be shifted by this quantity.

1. Exact eigenenergies

   •The ground state is the lowest singlet state s0: $E_{\text{exact,s0}} = \frac{U}{2}\left(1 - \sqrt{1 + \left(\frac{4t}{U}\right)^2}\right)$

   $$\begin{cases} \lim_{t\to 0} \; E_{\text{exact,s0}} & = & -\frac{4t^2}{U} \\ \lim_{t\to +\infty} \; E_{\text{exact,s0}} & = & \frac{U}{2} - 2t - \frac{U^2}{16t} \end{cases}$$

   • The highest eigenstate is the singlet s2: $E_{\text{exact,s2}} = \frac{U}{2}\left(1 + \sqrt{1 + \left(\frac{4t}{U}\right)^2}\right)$

   $$\begin{cases} \lim_{t\to 0} \; E_{\text{exact,s2}} & = & U + \frac{4t^2}{U} \\ \lim_{t\to +\infty} \; E_{\text{exact,s2}} & = & \frac{U}{2} + 2t + \frac{U^2}{16t} \end{cases}$$

   • The first excited singlet, s1, has an energy that is t-independent: $E_{\text{exact,s3}} = U$
   • The triplet energy t0 is also t-independent: $E_{\text{exact,t0}} = 0$

2. RHF solution
   • The approximated gound-state energy is: $E_{\mathrm{RHF}} = \frac{U}{2} - 2t$

   The $t = 0$ correponds to dissociation of the molecule. The RHF fails miserably in this case. The small U limit (large t limit) is instead correctly described.

3. UHF solution
   • We obtain the following solution depending on the t/U ratio:

$$\begin{cases} E_{\mathrm{UHF}} & = \frac{U}{2} - 2t = E_{\mathrm{RHF}} \quad \text{for} \quad 2t > U \\ E_{\mathrm{UHF}} & = -\frac{2t^2}{U} \qquad\qquad\qquad\quad \text{for} \quad 2t \leq U \end{cases}$$

   The unrestricted solution corrects the problem encountered by the restricted solution in the $t = 0$ case.
   However in the $t \to 0$ the energy of UHF is still a factor of 2 wrong if we take as reference the spacing between the singlet and triplet energy.
   Indeed in the $t \to 0$ limit, the UHF can be written as linear combination of s0 and t0:

$$\Psi_{\mathrm{UHF}} = \frac{1}{\sqrt{2}}\Psi_{\mathrm{exact,s0}} + \frac{1}{\sqrt{2}}\Psi_{\mathrm{exact,t0}}.$$