Consider a H_2 molecule immersed in a constant electric field, E, oriented along the direction of the bond between the two H atoms. This system can be described by a tight-binding model with the H $1s$ orbital as basis set and γ as hopping integral. The electric field produces a shift of the on-site energies of the two H atoms, so that they become $\epsilon_1 = \epsilon_0 + \delta$ and $\epsilon_2 = \epsilon_0 - \delta$ respectively for the first and the second H atom. δ is proportional to the electric field strength.

1. Calculate the tight-binding expression for the density matrix, ρ, associated to such a molecule when $\gamma = -1$, δ has a positive (non-zero) value and the molecule contains 2 electrons.
2. Demonstrate that the density matrix calculated in 1) has the property $\mathrm{Tr}[\rho] = 2$ regardless of the value of δ. Explain the physical meaning of such equality.
3. Calculate the density matrix for 2 electrons in the case of vanishing electric field ($\delta = 0$), and compare your results with those obtained previously in 1) in the limit $\delta \to 0$.
4. The polarizability of a molecule is defined as the derivative of the electrical dipole with respect to the electric field, evaluated at zero electric field. If one assumes that the H_2 bond length is 1 and so is the electron charge, then the electrical dipole operator of the H_2 molecule is defined as

$$\hat{P} = \frac{1}{2}[|1\rangle\langle 1| - |2\rangle\langle 2|]$$

where $|j\rangle\langle j|$ is the projector over the $1s$ atomic orbital centered on the j-th atom. By using the previously calculated density matrix evaluate the polarizability of the H_2 molecule (in the calculation assume that the electric field E is simply $E = c\delta$, with c a generic constant).