

H_2^+ Simulation

Aidan Macdonald

September 25, 2016

1 Equations

Hamiltonian for quantum mechanical electron and classical protons

$$\hat{H} = \frac{p_1^2 + p_2^2}{2M_p} + \frac{\hat{P}_e^2}{2m_e} + \frac{k}{\|q_1 - q_2\|} - \frac{k}{\|\hat{Q}_e - q_2\|} - \frac{k}{\|\hat{Q}_e - q_1\|}$$

Let $|\psi\rangle \triangleq |\psi_u\rangle + i|\psi_v\rangle$, then equations of motion are,

$$\begin{aligned}\dot{q}_1 &= p_1/M_p \\ \dot{q}_2 &= p_2/M_p \\ \dot{p}_1 &= \frac{-k(q_1 - q_2)}{\|q_1 - q_2\|^3} + \langle\psi|\frac{k(q_1 - \hat{Q}_e)}{\|q_1 - \hat{Q}_e\|^3}|\psi\rangle \\ \dot{p}_2 &= \frac{-k(q_2 - q_1)}{\|q_2 - q_1\|^3} + \langle\psi|\frac{k(q_2 - \hat{Q}_e)}{\|q_2 - \hat{Q}_e\|^3}|\psi\rangle \\ |\dot{\psi}_u\rangle &= \hat{H}|\psi_v\rangle \\ |\dot{\psi}_v\rangle &= -\hat{H}|\psi_u\rangle\end{aligned}$$