

# Quantum Chemistry

## Seminar 5

Approximate methods I

Variational methods

### Exercise 1 (Shamal)

Prove the equalities given on page 3 of lesson 5,  $\langle \psi | \psi \rangle = \sum_{k=0}^{+\infty} |c_k|^2$  and  $\langle \psi | \hat{H} | \psi \rangle = \sum_{k=0}^{+\infty} E_k |c_k|^2$ , provided that the Hamiltonian eigenfunctions,  $|\varphi_k\rangle$ , are orthonormal,  $\langle \varphi_j | \varphi_k \rangle = \delta_{jk}$ .

### Exercise 2 (Anila)

Show that  $|\psi(\tau)\rangle = \sum_{k=0}^{+\infty} c_{k0} e^{-\frac{E_k \tau}{\hbar}} |\varphi_k\rangle$ , where  $\hat{H} |\varphi_k\rangle = E_k |\varphi_k\rangle$ , represents a solution of the imaginary-time Schrödinger equation,  $\hat{H} |\psi(\tau)\rangle = -\hbar \frac{\partial |\psi(\tau)\rangle}{\partial \tau}$ .