Optimisation des grands systèmes

César Arnould - Victor Bertret - Antoine Gicquel - Hugo Tessier

4GM - INSA Rennes

Table des matières

Exercice 1: Comparaison des algorithmes

1.1 Question 1 :

The Schrödinger equation can describe the state of any quantum system :

$$t > 0, \quad i\hbar\frac{\partial\Psi}{\partial t}(x,t) = \Big(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\Big)\Psi(x,t) = E\Psi(x,t) \tag{1.1}$$

By using the separation of variables method we obtain the following expression for the wave function :

$$\forall x, \forall t \geq 0 : \Psi(x,t) = \phi(x)\nu(t) \Rightarrow \frac{\partial\Psi}{\partial t}(x,t) = \phi(x)\nu'(t) \; and \; \frac{\partial^2\Psi}{\partial x^2}(x,t) = \phi''(x)\nu(t)$$

By substituting in the Schrödinger equation, we find that :

$$\underbrace{-\frac{\hbar^2}{2m}\frac{\phi''(x)}{\phi(x)} + V(x)}_{X} = \underbrace{i\hbar\frac{\nu'(t)}{\nu(t)}}_{T}$$

X only depends on the space variable x, and T only depends on the time variable t. And since $X = T$, we have $X = T = E$, with E a constant that is homogeneous to an energy (same unit as $V(x)$).
By solving $i\hbar\frac{\nu'(t)}{\nu(t)} = E$, we have that $\nu(t) = A \ e^{-i\frac{E}{\hbar}t}$, with A a constant that is independent from t, so we can integrate it to $\phi(x)$.