# 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 $\phi(x)$.

# Exercice 2: Comparaison des algorithmes

## 2.1 Question 1 :

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

$$t > 0, \quad i\hbar \frac{\partial \Psi}{\partial t}(x,t) = \Big( - \frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \Big) \Psi(x,t) = E\Psi(x,t) \tag{2.1}$$

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 $\phi(x)$.

# Exercice 3: Comparaison des algorithmes

## 3.1 Question 1 :

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

$$t > 0, \quad i\hbar \frac{\partial \Psi}{\partial t}(x,t) = \Big( - \frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \Big) \Psi(x,t) = E\Psi(x,t) \tag{3.1}$$

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 $\phi(x)$.

# Exercice 4: Comparaison des algorithmes

## 4.1 Question 1 :

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

$$t > 0, \quad i\hbar\frac{\partial \Psi}{\partial t}(x,t) = \Big( -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\Big)\Psi(x,t) = E\Psi(x,t) \tag{4.1}$$

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 $\phi(x)$.