# CS 506
## Schrödinger's Wave Equation, Unitarity, and Measurement

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## 1 Schrödinger's (Non-Relativistic) Wave Equation

The Schrödinger wave equation is the fundamental equation governing how quantum states evolve over time. It is *non-relativistic*, meaning it assumes the velocity of the particle is small compared to the speed of light.

The Hamiltonian $H(t)$ represents the total energy of the system. It is a **Hermitian matrix**, satisfying

$$H(t)^\dagger = H(t).$$

The time-dependent Schrödinger equation is

$$i\,\hbar\,\frac{d\,|\psi(t)\rangle}{dt} \;=\; H(t)\;|\psi(t)\rangle\,. \tag{1}$$

Dividing both sides by $i\,\hbar$, we obtain

$$\begin{aligned}\frac{d\,|\psi(t)\rangle}{dt} &= \frac{1}{i}\,\frac{H(t)}{\hbar}\;|\psi(t)\rangle \\ &= -\,i\,\frac{H(t)}{\hbar}\;|\psi(t)\rangle\,. \end{aligned}\tag{2}$$

### 1.1 Time-Independent Hamiltonian

If $t_1 \approx t_2$, then $H(t_1) \approx H(t_2)$. We assume that $H(t)$ is **time-independent**, writing simply $H$ instead of $H(t)$. The equation becomes

$$\frac{d\,|\psi(t)\rangle}{dt} \;=\; -\,i\,\frac{H}{\hbar}\;|\psi(t)\rangle\,. \tag{3}$$

### 1.2 Solving the Equation

Equation (3) is an ordinary differential equation analogous to the scalar equation

$$\frac{d\,f(x)}{dx} = -\lambda\,f(x), \qquad f(x) = e^{-\lambda x}.$$

By direct analogy, the solution to the Schrödinger equation with time-independent Hamiltonian is

$$\boxed{|\psi(t_2)\rangle \;=\; e^{-\,i\,\frac{H}{\hbar}(t_2-t_1)}\;|\psi(t_1)\rangle} \tag{4}$$

The operator $U = e^{-\,i\,\frac{H}{\hbar}(t_2-t_1)}$ is a **unitary matrix**. Why?

## 2 Proof That the Time-Evolution Operator Is Unitary

Define $\lambda = -\frac{t_2 - t_1}{\hbar}$ so that $U = e^{i\lambda H}$. Since $H = H^\dagger$ (Hermitian), we also have $H^n = (H^\dagger)^n$ for all $n$.

### 2.1 Taylor Expansion of $U$

Using the matrix exponential (Taylor series):

$$\begin{aligned} U &= e^{i\lambda H} \\ &= I + \lambda i H + \frac{(\lambda i H)^2}{2!} + \frac{(\lambda i H)^3}{3!} + \frac{(\lambda i H)^4}{4!} + \cdots \\ &= I + \lambda i H + \frac{\lambda^2 i^2 H^2}{2!} + \frac{\lambda^3 i^3 H^3}{3!} + \frac{\lambda^4 i^4 H^4}{4!} + \cdots \end{aligned} \tag{5}$$

### 2.2 Taylor Expansion of $U^\dagger$

Taking the conjugate transpose:

$$\begin{aligned} U^\dagger &= \left(e^{i\lambda H}\right)^\dagger \\ &= I + \lambda(-i)H + \frac{\lambda^2(-i)^2(H^\dagger)^2}{2!} + \frac{\lambda^3(-i)^3(H^\dagger)^3}{3!} + \frac{\lambda^4(-i)^4(H^\dagger)^4}{4!} + \cdots \\ &= I + \lambda(-i)H + \frac{\lambda^2 i^2 H^2}{2!} + \frac{\lambda^3(-i^3)H^3}{3!} + \frac{\lambda^4 i^4 H^4}{4!} + \cdots \\ &= I - \lambda i H + \frac{\lambda^2 i^2 H^2}{2!} - \frac{\lambda^3 i^3 H^3}{3!} + \frac{\lambda^4 i^4 H^4}{4!} - \cdots \\ &= e^{-\lambda i H}. \end{aligned} \tag{6}$$

### 2.3 Showing $UU^\dagger = I$

Now we compute:

$$\begin{aligned} UU^\dagger &= e^{\lambda i H} \cdot e^{-\lambda i H} \\ &= e^{\lambda i (H - H)} \\ &= e^{\lambda i \cdot \mathbf{0}} \qquad \text{(matrix of all zeros)} \\ &= I + \lambda i\, \mathbf{0} + \frac{\lambda^2 i^2}{2!}\, \mathbf{0}^2 + \frac{\lambda^3 i^3}{3!}\, \mathbf{0}^3 + \cdots \\ &= I. \end{aligned} \tag{7}$$

Therefore $U = e^{i\lambda H}$ is unitary, and quantum time-evolution preserves probability.

## 3 Measurement (Observation) Postulate

### 3.1 Measurement in the Standard Basis

Given a quantum state

$$|\psi\rangle = \alpha_0\, |0\rangle + \alpha_1\, |1\rangle\,,$$

when we measure $|\psi\rangle$ in the standard (computational) basis $\{|0\rangle, |1\rangle\}$:

- $|\psi\rangle$ becomes $|0\rangle$ with probability $|\alpha_0|^2$,
- $|\psi\rangle$ becomes $|1\rangle$ with probability $|\alpha_1|^2$.

### 3.2 Example 1: Real Coefficients

Consider the state

$$|\psi\rangle = \underbrace{\frac{1}{\sqrt{3}}}_{\alpha_0} |0\rangle + \underbrace{\frac{\sqrt{2}}{\sqrt{3}}}_{\alpha_1} |1\rangle .$$

Measuring $|\psi\rangle$ in the basis $\{|0\rangle, |1\rangle\}$:

- $|\psi\rangle$ becomes $|0\rangle$ with probability $\left(\frac{1}{\sqrt{3}}\right)^2 = \frac{1}{3} = |\alpha_0|^2$,
- $|\psi\rangle$ becomes $|1\rangle$ with probability $\left(\frac{\sqrt{2}}{\sqrt{3}}\right)^2 = \frac{2}{3} = |\alpha_1|^2$.

### 3.3 Example 2: Complex Coefficients

Consider the state

$$|\psi\rangle = \underbrace{\left(\frac{1}{\sqrt{6}} + i\,\frac{\sqrt{5}}{\sqrt{6}}\right)}_{\alpha_0} |0\rangle \;+\; \underbrace{\left(\frac{1}{2} + i\,\frac{1}{2}\right)}_{\alpha_1} |1\rangle .$$

The measurement probabilities are:

$$|\alpha_0|^2 = \left(\frac{1}{\sqrt{6}}\right)^2 + \left(\frac{\sqrt{5}}{\sqrt{6}}\right)^2 = \frac{1}{6} + \frac{5}{6} = 1 \quad \text{(but see normalization below).}$$

$$|\alpha_1|^2 = \left(\frac{1}{2}\right)^2 + \left(\frac{1}{2}\right)^2 = \frac{1}{4} + \frac{1}{4} = \frac{1}{2}.$$

Measuring $|\psi\rangle$ in the basis $\{|0\rangle, |1\rangle\}$:

- $|\psi\rangle$ becomes $|0\rangle$ with probability $|\alpha_0|^2 = \frac{1}{2}$,
- $|\psi\rangle$ becomes $|1\rangle$ with probability $|\alpha_1|^2 = \frac{1}{2}$.

## 4 Measurement in the Hadamard Basis

### 4.1 Hadamard Basis States

The Hadamard (plus/minus) basis is given by

$$|+\rangle = \frac{1}{\sqrt{2}} |0\rangle + \frac{1}{\sqrt{2}} |1\rangle , \tag{8}$$

$$|-\rangle = \frac{1}{\sqrt{2}} |0\rangle - \frac{1}{\sqrt{2}} |1\rangle . \tag{9}$$

We can invert these relations to express the computational basis in terms of the Hadamard basis:

$$|0\rangle = \frac{1}{\sqrt{2}}\ |+\rangle + \frac{1}{\sqrt{2}}\ |-\rangle\,, \tag{10}$$

$$|1\rangle = \frac{1}{\sqrt{2}}\ |+\rangle - \frac{1}{\sqrt{2}}\ |-\rangle\,. \tag{11}$$

*Derivation.* Adding and subtracting the Hadamard states:

$$|+\rangle + |-\rangle = \frac{2}{\sqrt{2}}\ |0\rangle\,, \qquad \frac{1}{\sqrt{2}}(|+\rangle + |-\rangle) = |0\rangle\,.$$

### 4.2 Rewriting $|\psi\rangle$ in the Hadamard Basis

Taking the state from Example 2:

$$|\psi\rangle = \left(\frac{1}{\sqrt{6}} + i\,\frac{\sqrt{5}}{\sqrt{6}}\right)|0\rangle + \left(\frac{1}{2} + \frac{1}{2}\,i\right)|1\rangle\,,$$

and substituting $|0\rangle$ and $|1\rangle$ in terms of $|+\rangle$ and $|-\rangle$:

$$|\psi\rangle = \left(\frac{1}{\sqrt{6}} + i\,\frac{\sqrt{5}}{\sqrt{6}}\right)\left(\frac{1}{\sqrt{2}}\,|+\rangle + \frac{1}{\sqrt{2}}\,|-\rangle\right) + \left(\frac{1}{2} + \frac{1}{2}\,i\right)\left(\frac{1}{\sqrt{2}}\,|+\rangle - \frac{1}{\sqrt{2}}\,|-\rangle\right). \tag{12}$$

Expanding and collecting terms:

$$\begin{aligned}|\psi\rangle &= \frac{1}{\sqrt{12}}\,|+\rangle + \frac{1}{\sqrt{12}}\,|-\rangle + \frac{i}{\sqrt{6}}\,|+\rangle + \frac{i\sqrt{5}}{\sqrt{12}}\,|-\rangle \\ &\quad + \frac{1}{2\sqrt{2}}\,|+\rangle - \frac{1}{2\sqrt{2}}\,|-\rangle + \frac{i}{2\sqrt{2}}\,|+\rangle - \frac{i}{2\sqrt{2}}\,|-\rangle\,.\end{aligned} \tag{13}$$

Grouping:

$$|\psi\rangle = \underbrace{\left[\left(\frac{1}{\sqrt{12}} + \frac{1}{2\sqrt{2}}\right) + i\left(\frac{1}{\sqrt{6}} + \frac{1}{2\sqrt{2}}\right)\right]}_{\alpha}|+\rangle \;+\; \underbrace{\left[\left(\frac{1}{\sqrt{12}} - \frac{1}{2\sqrt{2}}\right) + i\left(\frac{1}{\sqrt{6}} - \frac{1}{2\sqrt{2}}\right)\right]}_{\beta}|-\rangle\,. \tag{14}$$

Measuring $|\psi\rangle$ in the Hadamard basis:

- $|\psi\rangle$ becomes $|+\rangle$ with probability $|\alpha|^2 = \left(\frac{1}{\sqrt{12}} + \frac{1}{2\sqrt{2}}\right)^2 + \left(\frac{1}{\sqrt{6}} + \frac{1}{2\sqrt{2}}\right)^2$,
- $|\psi\rangle$ becomes $|-\rangle$ with probability $|\beta|^2 = \left(\frac{1}{\sqrt{12}} - \frac{1}{2\sqrt{2}}\right)^2 + \left(\frac{1}{\sqrt{6}} - \frac{1}{2\sqrt{2}}\right)^2$.

# 5 Multi-Qubit Measurement

### 5.1 2-Qubit State and Standard Basis Measurement

Consider a 2-qubit state:

$$|\psi\rangle = \frac{1}{\sqrt{11}}\ |00\rangle + \frac{\sqrt{5}}{\sqrt{11}}\ |01\rangle + \frac{\sqrt{2}}{\sqrt{11}}\ |10\rangle + \frac{\sqrt{3}}{\sqrt{11}}\ |11\rangle\,.$$

Here the first entry in each ket labels the **1st qubit** and the second entry labels the **2nd qubit**. Measuring both qubits in the standard basis $\{|00\rangle\,, |01\rangle\,, |10\rangle\,, |11\rangle\}$:

- $|\psi\rangle$ becomes $|00\rangle$ with probability $\left(\frac{1}{\sqrt{11}}\right)^2 = \frac{1}{11}$,
- $|\psi\rangle$ becomes $|01\rangle$ with probability $\left(\frac{\sqrt{5}}{\sqrt{11}}\right)^2 = \frac{5}{11}$,
- $|\psi\rangle$ becomes $|10\rangle$ with probability $\left(\frac{\sqrt{2}}{\sqrt{11}}\right)^2 = \frac{2}{11}$,
- $|\psi\rangle$ becomes $|11\rangle$ with probability $\left(\frac{\sqrt{3}}{\sqrt{11}}\right)^2 = \frac{3}{11}$.

### 5.2 Partial Measurement: Measuring Only the 1st Qubit

What if we want to measure only the 1st qubit?

We rewrite the state by factoring out the 1st qubit:

$$\begin{aligned} |\psi\rangle &= \alpha_{00}\,|00\rangle + \alpha_{01}\,|01\rangle + \alpha_{10}\,|10\rangle + \alpha_{11}\,|11\rangle \\ &= \beta_0\;|0\rangle\,(\gamma_0\,|0\rangle + \gamma_1\,|1\rangle) + \beta_1\;|1\rangle\,(\gamma_0'\,|0\rangle + \gamma_1'\,|1\rangle). \end{aligned} \tag{15}$$

Substituting the coefficients:

$$|\psi\rangle = \frac{\sqrt{6}}{\sqrt{11}}\;|0\rangle\left(\frac{1}{\sqrt{6}}\,|0\rangle + \frac{\sqrt{5}}{\sqrt{6}}\,|1\rangle\right) + \frac{\sqrt{5}}{\sqrt{11}}\;|1\rangle\left(\frac{\sqrt{2}}{\sqrt{5}}\,|0\rangle + \frac{\sqrt{3}}{\sqrt{5}}\,|1\rangle\right). \tag{16}$$

When we measure **only the 1st qubit**:

- 1st qubit becomes $|0\rangle$ with probability $\left(\frac{\sqrt{6}}{\sqrt{11}}\right)^2 = \frac{6}{11} = \beta_0^2$.

  The 2nd qubit is then left in the state $\frac{1}{\sqrt{6}}\,|0\rangle + \frac{\sqrt{5}}{\sqrt{6}}\,|1\rangle$.
- 1st qubit becomes $|1\rangle$ with probability $\left(\frac{\sqrt{5}}{\sqrt{11}}\right)^2 = \frac{5}{11} = \beta_1^2$.

  The 2nd qubit is then left in the state $\frac{\sqrt{2}}{\sqrt{5}}\,|0\rangle + \frac{\sqrt{3}}{\sqrt{5}}\,|1\rangle$.

After partial measurement, the overall state collapses to one of:

$$|0\rangle\left(\frac{1}{\sqrt{6}}\,|0\rangle + \frac{\sqrt{5}}{\sqrt{6}}\,|1\rangle\right) \qquad \text{or} \qquad |1\rangle\left(\frac{\sqrt{2}}{\sqrt{5}}\,|0\rangle + \frac{\sqrt{3}}{\sqrt{5}}\,|1\rangle\right).$$

# 6 Bell Basis and Entanglement

## 6.1 The Bell Basis

The **Bell basis** is an important two-qubit orthonormal basis. The four Bell states (also called **EPR pairs**) are:

$$|\beta_{00}\rangle = \frac{1}{\sqrt{2}}\,|00\rangle + \frac{1}{\sqrt{2}}\,|11\rangle\,, \tag{17}$$

$$|\beta_{01}\rangle = \frac{1}{\sqrt{2}}\,|01\rangle + \frac{1}{\sqrt{2}}\,|10\rangle\,, \tag{18}$$

$$|\beta_{10}\rangle = \frac{1}{\sqrt{2}}\,|00\rangle - \frac{1}{\sqrt{2}}\,|11\rangle\,, \tag{19}$$

$$|\beta_{11}\rangle = \frac{1}{\sqrt{2}}\,|01\rangle - \frac{1}{\sqrt{2}}\,|10\rangle\,. \tag{20}$$

## 6.2 Entanglement

Consider the Bell state $|\beta_{00}\rangle$:

$$\frac{1}{\sqrt{2}}\,|00\rangle + \frac{1}{\sqrt{2}}\,|11\rangle\,.$$

Can we measure only the 1st qubit? That would require writing this state in the factored form

$$\beta_0\,|0\rangle\,(\gamma_0\,|0\rangle + \gamma_1\,|1\rangle) + \beta_1\,|1\rangle\,(\gamma_0'\,|0\rangle + \gamma_1'\,|1\rangle).$$

This is **not possible** for any choice of $\beta_0, \gamma_0, \gamma_1, \beta_1, \gamma_0', \gamma_1'$. That is, the Bell state $|\beta_{00}\rangle$ cannot be written as a product of two single-qubit states.

When a two-qubit state cannot be factored in this way, the two qubits are said to be **"entangled."**