

Introduction to Superconducting Quantum Circuits

- Review of Mathematical Methods for Quantum Computing -

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Lecture Overview

Week 1. Introduction to Superconducting Quantum Circuits

Week 2. Review of Mathematics and Microwave Engineering

Week 3. Review of Classical and Quantum Mechanics

Week 4. Review of Superconductivity

Week 5. Quantum Harmonic/Anharmonic Oscillators and Light-Matter Interaction

Week 6. Circuit Quantization Methods

Week 7. Parametrically Pumped Josephson Devices

Week 8. Design and Analysis of Superconducting Resonators

Week 9. Design and Analysis of Superconducting Qubits

Week 10. Design and Analysis of Single-Qubit Device: 3D Cavity

Week 11. Design and Analysis of Single-Qubit Device : 2D Chip

Week 12. Design and Analysis of Two-Qubit Device

Week 13. Design and Analysis of Josephson Parametric Amplifier

Week 14. Term Project

Week 15. Term Project

overall backgrounds, terminologies
of quantum computing

mathematical and engineering backgrounds
general superconductivity

Quantum circuit analysis

design and analysis of superconducting RF devices

Keywords in Mathematical Methods for Quantum Computing

Mathematical Methods: Number Systems

Complex Number Polar Coordinates Euler Expressions

Mathematical Methods: Series Expansion

Taylor Expansion Jacobi-Anger Expansion Fourier Series Fourier Transform

Mathematical Methods: Linear Algebra

Hilbert Space Bra-Ket Notation Dirac Notation

Adjoint Operation Linear Operator Unitary Operator Hermitian Operator

Inner Product Tensor Product Taylor Expansion of Operators

Basis State Kronecker Delta Levi-Civita Eigenvalue Eigenstate

Mathematical Methods: Differential Equation

Ordinary Differential Equation Partial Differential Equation Green's Function

Mathematical Methods: Vector Calculus

Divergence Theorem Stokes' Theorem

Mathematical Methods: Dimensional Analysis

Physical Unit Conversion

Introduction to Number Systems

■ Major Number Systems

- Natural numbers: $\mathbb{N} = \{1, 2, 3, \dots\}$
- Integers: $\mathbb{Z} = \{\dots, -3, -2, -1, 0, 1, 2, 3, \dots\}$
- Rational numbers: $\mathbb{Q} = \{\frac{a}{b}\}$ where a and b are integers
- Irrational numbers: \mathbb{I} where elements can NOT be expressed with $\frac{a}{b}$
- Real numbers: $\mathbb{R} = \mathbb{Q} \cup \mathbb{I} = \{x: x \in \mathbb{Q} \text{ or } x \in \mathbb{I}\}$
- Complex numbers: $\mathbb{C} = \{a + bj\}$ where a and b are real

NOTE: all quantum states are expressed with complex numbers

■ Number System Set Inclusions

- $\mathbb{N} \subset \mathbb{Z} \subset \mathbb{Q} \subset \mathbb{R} \subset \mathbb{C}$

■ Imaginary Unit (j)

- The imaginary unit is a solution of $x^2 = -1$
- $1i = \sqrt{-1}$ (which is same as $1j = \sqrt{-1}$)

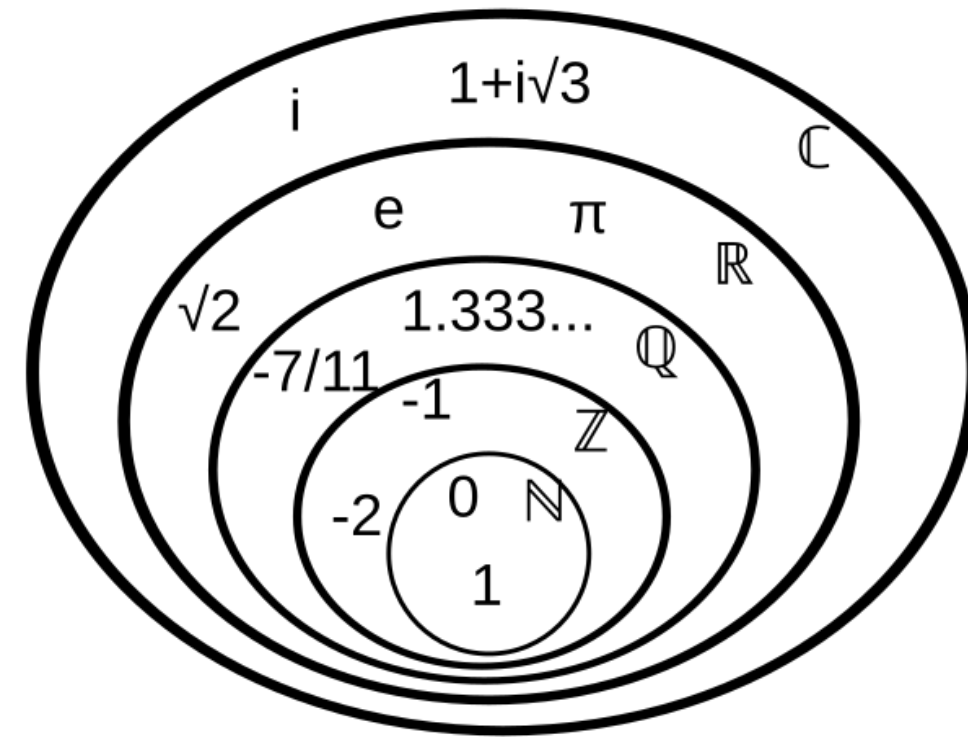


Figure. Number system set diagram

NOTE

most of electrical engineers prefer $1j$ notation rather than $1i$, since i is used to denote the electrical current

Brief Review of Number Systems: Complex Number Expressions

- Complex Numbers: Real Part + Imaginary Part

$$z = a + bj \longleftrightarrow z^* = a - bj \text{ (conjugate of } z\text{)}$$

- Polar Coordinates for Complex Numbers

$$z = (r, \theta)$$

where
 $r = \sqrt{a^2 + b^2}$ and $\theta = \arctan(\frac{b}{a})$

- Euler Expressions for Complex Numbers

$$z = r e^{j\theta}$$

where Euler's formula is
 $e^{j\theta} = \cos \theta + j \sin \theta$
Euler's identity is
 $e^{j\pi} + 1 = 0$

- Example: $z = 2 + 2\sqrt{3}j$

$$z = 2 + 2\sqrt{3}j \rightarrow r = \sqrt{2^2 + (2\sqrt{3})^2} = 4 \text{ and } \theta = \arctan\left(\frac{2\sqrt{3}}{2}\right) = \frac{\pi}{3} \rightarrow z = 4e^{j\frac{\pi}{3}}$$

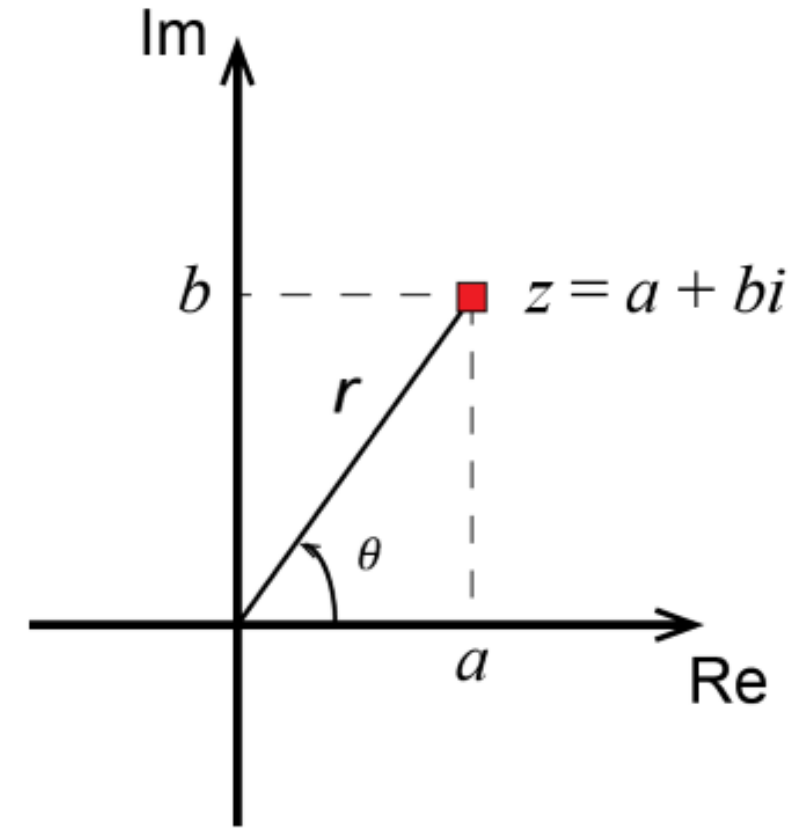


Figure. Polar form of a complex number $z = a + bj$

Brief Review of Series Expansion: (1) Taylor Expansion

■ Definition of Taylor Expansion

- Approximation of a function $f(x)$ as a series of infinite sum of polynomial terms

■ Formula of Taylor Expansion

- For a function $f(x)$ that is **infinitely differentiable at $x = a$** , the Taylor series expansion **around a** is:

$$f(x) = f(a) + f'(a)(x - a) + \frac{f''(a)}{2!}(x - a)^2 + \frac{f'''(a)}{3!}(x - a)^3 + \dots$$

in simplified notation:

$$f(x) = \sum_{n=0}^{\infty} \frac{1}{n!} \frac{d^n}{dx^n} f(x) \Big|_{x=a} (x - a)^n$$

where $n!$ is factorial
 $n! = 1 \times 2 \times \dots \times n - 1 \times n$

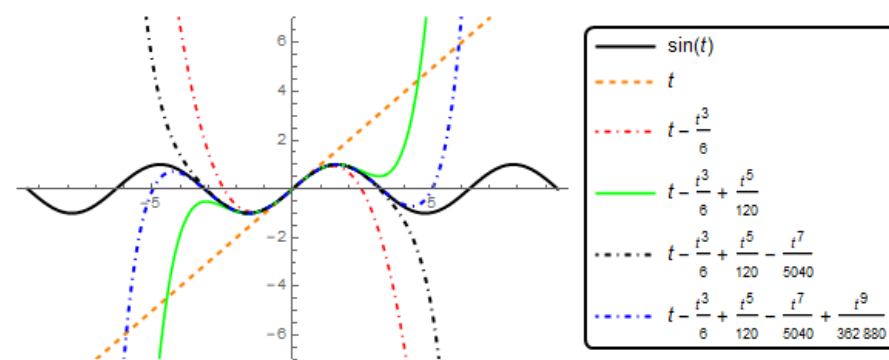


Figure. Truncated Taylor series of sine function up to 9th order

■ Truncation of Taylor Expansion

- In reality, infinite sum of Taylor series can not be computed...
- For simplicity, **only few low-order terms are only considered in practice**

■ Example $f(\theta) = \cos \theta$ around $\theta = 0$

$$f(\theta) = \sum_{n=0}^{\infty} \frac{1}{n!} \frac{d^n}{d\theta^n} \cos \theta \Big|_{\theta=0} \theta^n = 1 - \frac{\theta^2}{2!} + \frac{\theta^4}{4!} - \frac{\theta^6}{6!} + \dots$$

Brief Review of Series Expansion: (2) Jacobi-Anger Expansion

■ Definition of Jacobi-Anger Expansion

- Approximation of an exponential function with trigonometric terms as a series of infinite sum of Bessel functions

■ Formula of Jacobi-Anger Expansion

- For a function $e^{jx \cos \theta}$,

$$e^{jx \cos \theta} = \sum_{n=-\infty}^{\infty} j^n J_n(x) e^{jn\theta}$$

- For a function $e^{jx \sin \theta}$,

$$e^{jx \sin \theta} = \sum_{n=-\infty}^{\infty} J_n(x) e^{jn\theta}$$

where $J_n(x)$ is Bessel function of the first kind and $\Gamma(n)$ is Gamma function

$$J_n(x) = \sum_{m=0}^{\infty} \frac{(-1)^m}{m! \Gamma(m+n+1)} \left(\frac{x}{2}\right)^{2m+n} \quad \Gamma(n) = \int_0^{\infty} x^{n-1} e^{-x} dx$$

■ Some Useful Expressions of Jacobi-Anger Expansion

NOTE: these expressions will be utilized,
when we analyze Josephson junction after

$$\begin{aligned} \cos(z \cos \theta) &\equiv J_0(z) + 2 \sum_{n=1}^{\infty} (-1)^n J_{2n}(z) \cos(2n\theta), & \cos(z \sin \theta) &\equiv J_0(z) + 2 \sum_{n=1}^{\infty} J_{2n}(z) \cos(2n\theta), \\ \sin(z \cos \theta) &\equiv -2 \sum_{n=1}^{\infty} (-1)^n J_{2n-1}(z) \cos[(2n-1)\theta], & \sin(z \sin \theta) &\equiv 2 \sum_{n=1}^{\infty} J_{2n-1}(z) \sin[(2n-1)\theta]. \end{aligned}$$

Brief Review of Fourier Analysis: (1) Fourier Series

■ Definition of Fourier Series

- Approximation of a **periodic function** as a **sum of trigonometric terms**

■ Formula of Fourier Series

- For a function $f(t)$ with period $2l$,

$$f(t) = \sum_{n=-\infty}^{\infty} c_n e^{\frac{jn\pi t}{l}}$$

where c_n coefficient is

$$c_n = \frac{1}{2l} \int_{-l}^l f(t) e^{-\frac{jn\pi t}{l}} dx$$

■ Properties of Fourier Series

- For functions $f_1(t) = \sum a_n e^{\frac{jn\pi t}{l}}$ and $f_2(t) = \sum b_n e^{\frac{jn\pi t}{l}}$,
- Linearity: $a f_1(t) + b f_2(t) = a \left(\sum a_n e^{\frac{jn\pi t}{l}} \right) + b \left(\sum b_n e^{\frac{jn\pi t}{l}} \right)$
- Shift in time: $f_1(t - t_0) = \left(\sum a_n e^{\frac{jn\pi(t-t_0)}{l}} \right)$

■ Example $f(t) \begin{cases} 0, & 0 < x < 0.5 \\ 1, & 0.5 < x < 1 \end{cases}$ and its period 1

$$f(t) = \frac{1}{2} + \frac{1}{j\pi} \left(e^{2j\pi t} - e^{-2j\pi t} + \frac{1}{3} (e^{6j\pi t} - e^{-6j\pi t}) + \frac{1}{5} (e^{10j\pi t} - e^{-10j\pi t}) + \dots \right)$$

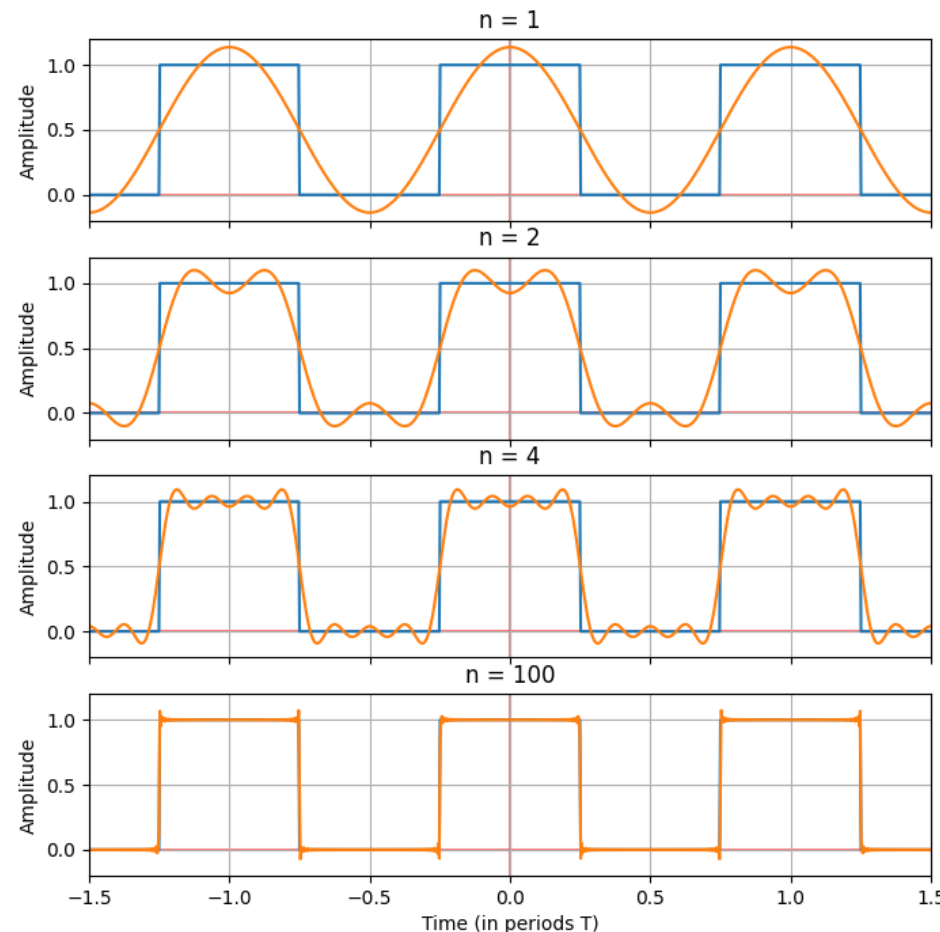


Figure. Fourier series approximation of squared pulse up to $N = 100$

Brief Review of Fourier Analysis: (2) Fourier Transform

■ Definition of Fourier Transform

- Conversion of an arbitrary time-domain signal $f(t)$ into its frequency-domain $F(\omega)$

■ Formula of Fourier Transform

- For a function $f(t)$, the transformed function $F(\omega)$ is

$$F(\omega) = \int_{-\infty}^{\infty} f(t) e^{-j\omega t} dt$$

■ Properties of Fourier Transform

- Linearity: $a f_1(t) + b f_2(t) \Leftrightarrow a F_1(\omega) + b F_2(\omega)$
- Time shifting: $f(t - t_0) \Leftrightarrow e^{-j t_0 \omega} F(\omega)$
- Time scaling: $f(at) \Leftrightarrow \frac{1}{|a|} F\left(\frac{\omega}{a}\right)$

■ Some Useful Examples of Fourier Transform

- square pulse in time domain \Leftrightarrow sinc in frequency domain
- Gaussian pulse in time domain \Leftrightarrow Gaussian (but different amplitude) in frequency domain
- Gaussian modulated cosine (frequency: ω_0) pulse in time domain \Leftrightarrow two Gaussian (with ω_0 and $-\omega_0$) in frequency domain

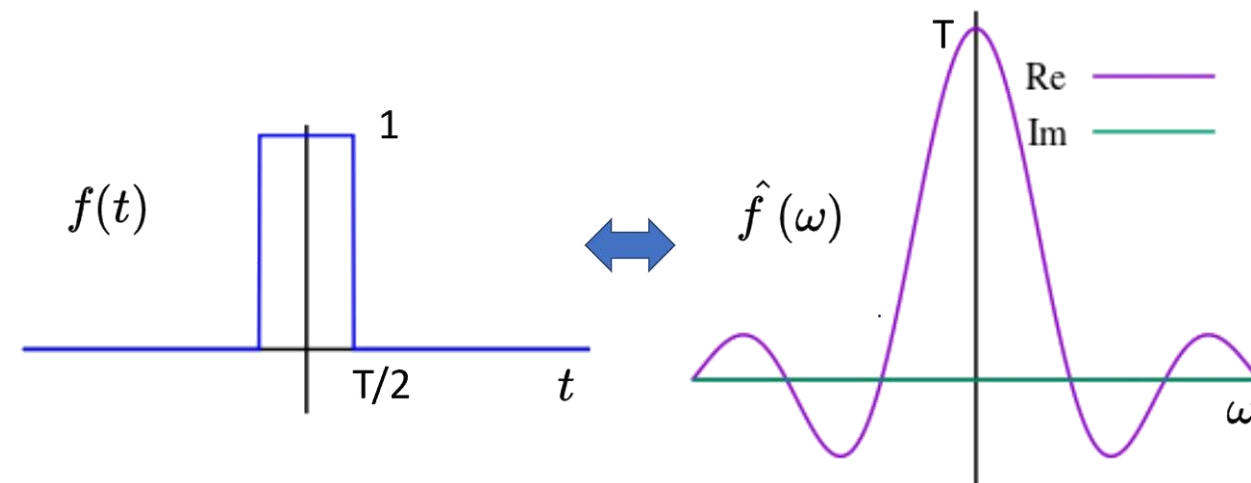


Figure. Square pulse in time domain and its Fourier transformed function in frequency domain

NOTE: these expressions are useful,
when we control a superconducting qubit with RF pulse

Brief Review of Linear Algebra: (1) Bra-Ket Notation (Dirac Notation)

■ Definition of Bra-Ket Notation (also Known as Dirac Notation)

- A standard notation for describing quantum states in the mathematical framework

■ Key Components of Bra-Ket Notation

- Ket vector $|\psi\rangle$: a column vector
- Bra vector $\langle\psi|$: a row vector, which is **conjugate transpose (symbol: \dagger , dagger)** of a Ket vector

$$\begin{array}{c} \text{Ket} \\ |\psi\rangle = \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{pmatrix} \end{array}$$

$$\begin{array}{c} \text{Bra} \\ \langle\psi| = |\psi\rangle^\dagger \\ = (a_1^*, a_2^*, \dots, a_n^*) \end{array}$$

■ Inner Product Using Bra-Ket Notation

$$\int \psi_a^* \psi_b = \langle\psi_a|\psi_b\rangle = (a_1^*, a_2^*, \dots, a_n^*) \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{pmatrix} = \sum_{i=1} a_i^* b_i$$

NOTE: inner product can be also expressed as $\langle\psi_a, \psi_b\rangle$ instead of $\langle\psi_a|\psi_b\rangle$

■ Why Do We Use Bra-Ket Notation?

- Simple notation to express the quantum state

Brief Review of Linear Algebra: (2) Inner Product

■ Definition of Inner Product

- The inner product (or dot product) in a Hilbert space returns scalar by multiplying two vectors

$$\langle \psi_a | \psi_b \rangle = (a_1^*, a_2^*, \dots, a_n^*) \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{pmatrix} = \sum_{i=1}^n a_i^* b_i$$

■ Properties of Inner Product

- Linearity: $\langle c_1 \psi_1 + c_2 \psi_2 | \psi_3 \rangle = c_1 \langle \psi_1 | \psi_3 \rangle + c_2 \langle \psi_2 | \psi_3 \rangle$

where c_1 and c_2 are scalar constants

- Conjugate symmetric: $\langle \psi_a | \psi_b \rangle = \langle \psi_b | \psi_a \rangle^*$

- Positive definite: $\langle \psi_a | \psi_a \rangle \geq 0$, with equality if and only if $\psi_a = 0$

■ Characteristics of Inner Product for Quantum Computing

- Inner product represents **projection of a quantum state** to the other state
- Square of inner product $|\langle \psi | \phi \rangle|^2$ indicates the **probability of a system** to be in state $|\psi\rangle$, given that the system is in state $|\phi\rangle$

■ Example of Inner Product

- For vectors $|\psi\rangle = \begin{pmatrix} 1 \\ i \end{pmatrix}$ and $|\phi\rangle = \begin{pmatrix} 2 \\ 1 \end{pmatrix}$, $\langle \psi | \phi \rangle = (1 \quad -i) \begin{pmatrix} 2 \\ 1 \end{pmatrix} = 2 - i$

Brief Review of Linear Algebra: (3) Tensor Product

■ Definition of Tensor Product

- The tensor product of two vector spaces V and W results in a new vector space, denoted $V \otimes W$
- For vectors $|\psi\rangle = \begin{pmatrix} a \\ b \end{pmatrix}$ in V and $|\phi\rangle = \begin{pmatrix} c \\ d \end{pmatrix}$ in W , the tensor product $|\psi\rangle \otimes |\phi\rangle$ is

$$|\psi\rangle \otimes |\phi\rangle = \begin{pmatrix} ac \\ ad \\ bc \\ bd \end{pmatrix}$$

■ Properties of Tensor Product

- Linearity: $(a|\psi_1\rangle + b|\psi_2\rangle) \otimes |\phi\rangle = a(|\psi_1\rangle \otimes |\phi\rangle) + b(|\psi_2\rangle \otimes |\phi\rangle)$
- Associativity: $(|\psi_1\rangle \otimes |\psi_2\rangle) \otimes |\psi_3\rangle = |\psi_1\rangle \otimes (|\psi_2\rangle \otimes |\psi_3\rangle)$

■ Characteristics of Tensor Product for Quantum Computing

- Tensor product represents **the combined state of two quantum systems**

■ Example of Tensor Product

- For qubit #1 in state $|0\rangle$ and qubit #2 in state $\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$, the tensor product of qubit #1 and qubit #2 is

$$|0\rangle \otimes \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \\ 0 \\ 0 \end{pmatrix}$$

Brief Review of Linear Algebra: (4) Hilbert Space

■ Definition of Hilbert Space

- Hilbert space is a **complete**, infinite-dimensional vector space equipped with an **inner product**

■ Properties of Hilbert Space

- Vector space: A collection of vectors where vector addition and scalar multiplication are defined
- Inner product: Dot product (integration over the entire vector space) of two vectors
- Orthogonality: two vectors $|\psi\rangle$ and $|\phi\rangle$ are orthogonal, if the inner product is zero $\langle\psi|\phi\rangle=0$
- Norm: length of a vector $|\psi\rangle$ is calculated as $\|\psi\| = \sqrt{\langle\psi|\psi\rangle}$
- Basis: Any vector in the Hilbert space can be expressed as a combination of the basis vectors

NOTE: Here, we consider a qubit as two-level system.

A qubit can be considered as m -level system for some cases.

■ Example of Hilbert Space

- Single qubit system: 2-dimensional space with basis $|0\rangle$ and $|1\rangle$
- Two qubit system: 4-dimensional space with basis $|00\rangle, |01\rangle, |10\rangle$, and $|11\rangle$
- n qubit system: 2^n -dimensional space with basis $|00 \cdots 00\rangle, |00 \cdots 01\rangle, \dots, |11 \cdots 11\rangle$

Brief Review of Linear Algebra: (5) Linear Operators

■ Definition of Linear Operator

- A mapping function \hat{L} between two vector spaces
- In typical quantum computing problems, a linear operator \hat{L} maps two vectors within the same Hilbert space

■ Properties of Linear Operator

- Linearity: $\hat{L}(a|\psi\rangle + b|\phi\rangle) = a\hat{L}|\psi\rangle + b\hat{L}|\phi\rangle$
- Associativity: $\langle\psi|\hat{L}|\phi\rangle = \langle(\psi\hat{L})|\phi\rangle = \langle\psi|(\hat{L}\phi)\rangle$

where a and b are scalar constants

■ Characteristics of Linear Operator for Quantum Computing

- In a finite-dimensional Hilbert space, linear operators can be represented as matrices
- For a Ket vector in a n -dimensional space, a linear operator \hat{L} can be represented by an $n \times n$ matrix

■ Example of Linear Operator

- Qubit NOT gate (also known as Pauli X gate): flips qubit state between $|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $|1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$
- Matrix representation of the NOT gate: $\hat{X} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ that $\hat{X}|0\rangle = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} = |1\rangle$ and vice versa

Brief Review of Linear Algebra: (6) Basis States

■ Definition of Basis States

- Basis is a set of linearly independent vectors that span a vector space

■ Properties of Basis States

- Orthogonality: Basis states are orthogonal, meaning $\langle 0|1\rangle=0$ and $\langle 1|0\rangle=0$
- Normalization: Basis states are normalized, meaning $\langle 0|0\rangle=1$ and $\langle 1|1\rangle=1$
- Superposition: Any state $|\psi\rangle$ can be expressed as a linear combination of basis states

■ Characteristics of Basis States for Quantum Computing

- A qubit's state can be represented by a **superposition of basis states $|0\rangle$ and $|1\rangle$** as $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$
- Measuring a qubit in superposition collapses it to one of the basis states, $|0\rangle$ or $|1\rangle$, with probabilities of $|\alpha|^2$ or $|\beta|^2$
- Otherwise, one can define qubit's basis states with **$|+\rangle$ and $|-\rangle$** states
- A qubit's state can be represented by a **superposition of basis states $|+\rangle$ and $|-\rangle$** as $|\psi\rangle = \alpha|+\rangle + \beta|-\rangle$
- Measuring a qubit in superposition collapses it to one of the basis states, $|+\rangle$ or $|-\rangle$, with probabilities of $|\alpha|^2$ or $|\beta|^2$

$$\text{where } |+\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \text{ and } |-\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$$

Brief Review of Linear Algebra: (7) Kronecker Delta and Levi-Civita

■ Definition of Kronecker Delta

- The Kronecker delta, denoted as δ_{ij} , is a function of two variables (usually integers) that is 0 or 1, defined as

$$\delta_{ij} = \begin{cases} 0, & \text{if } i \neq j \\ 1, & \text{if } i = j \end{cases}$$

■ Definition of Levi-Civita

- The Levi-Civita, denoted as ε_{ijk} , is a function of three variables (usually integers) that is -1, 0 or 1, defined as

$$\varepsilon_{ijk} = \begin{cases} +1 & \text{if } (i, j, k) \text{ is } (1, 2, 3), (2, 3, 1), \text{ or } (3, 1, 2), \\ -1 & \text{if } (i, j, k) \text{ is } (3, 2, 1), (1, 3, 2), \text{ or } (2, 1, 3), \\ 0 & \text{if } i = j, \text{ or } j = k, \text{ or } k = i \end{cases}$$

- The generalized Levi-Civita in n -dimensions is defined as

$$\varepsilon_{a_1 a_2 a_3 \dots a_n} = \begin{cases} +1 & \text{if } (a_1, a_2, a_3, \dots, a_n) \text{ is an even permutation of } (1, 2, 3, \dots, n) \\ -1 & \text{if } (a_1, a_2, a_3, \dots, a_n) \text{ is an odd permutation of } (1, 2, 3, \dots, n) \\ 0 & \text{otherwise} \end{cases}$$

■ Why Do We Use Kronecker Delta and Levi-Civita?

- Simplified expressions of matrix operations

Brief Review of Linear Algebra: (8) Eigenvalues and Eigenstates

■ Definition of Eigenvalue

- The constant factor λ by which the eigenstate is scaled when the operator \hat{O} is applied

■ Definition of Eigenstate

- The quantum state $|\psi\rangle$ that, when an operator \hat{O} is applied to it, results in the state being scaled by its eigenvalue.

$$\hat{O}|\psi\rangle = \lambda|\psi\rangle$$



eigenstate
eigenvalue

■ Formula of Eigenvalues and Eigenstates

- For n -dimensional Hilbert space, \hat{O} is $n \times n$ matrix
- By solving the linear equation of $\det(\hat{O} - \lambda \hat{I}) = 0$, eigenvalues and eigenstates of the operator \hat{O} can be obtained

■ Example of Eigenvalues and Eigenstates

- For the Pauli-Z gate $\hat{Z} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$, eigenstate $|0\rangle$ and its corresponding $\lambda = 1$, while eigenstate $|1\rangle$ and its $\lambda = -1$

Brief Review of Linear Algebra: (9) Adjoint Operation

■ Definition of Adjoint Operation

- Adjoint of a linear operator \hat{A} , denoted as \hat{A}^\dagger : complex conjugate transpose of $\hat{A} \rightarrow \text{transpose}(\hat{A}^*)$

■ Formula of Adjoint Operation

- For $n \times n$ matrix \hat{A} , let the (i, j) element representation as \hat{A}_{ij}
- The (j, i) element of the \hat{A}^\dagger is $(\hat{A}^\dagger)_{ji} = (\hat{A}_{ij})^*$

■ Characteristics of Adjoint Operation

- The adjoint of a linear operator \hat{A} satisfies the following relation for all vectors in a Hilbert space:

$$\langle \psi | \hat{A} | \phi \rangle = \langle \psi | \hat{A} \phi \rangle = \langle \psi | \hat{A}^\dagger | \phi \rangle$$

- An operator \hat{A} is unitary operator, if $\hat{A}\hat{A}^\dagger = \hat{A}^\dagger\hat{A} = \hat{I}$
- An operator \hat{A} is Hermitian operator, if $\hat{A} = \hat{A}^\dagger$

Details of unitary and Hermitian operators
will be discussed next slides

■ Example of Adjoint Operation

- For an operator $\hat{A} = \begin{pmatrix} 2 & 1+j \\ -1 & 2-j \end{pmatrix}$, the adjoint $\hat{A}^\dagger = \begin{pmatrix} 2 & -1 \\ 1-j & 2+j \end{pmatrix}$

Brief Review of Linear Algebra: (10) Unitary Operators

■ Definition of Unitary Operator

- A linear operator \hat{U} is unitary, if it satisfies: $\hat{U}^\dagger \hat{U} = \hat{I}$, where \hat{I} is the identity operator

■ Properties of Unitary Operator

- Norm preservation: An unitary operator \hat{U} preserves the norm (length) of vectors
- Reversibility: An unitary operator \hat{U} is reversible that its inverse \hat{U}^{-1} exists and is defined as $\hat{U}^{-1} = \hat{U}^\dagger$
- Inner product preservation: An unitary operator \hat{U} preserves the inner product as $\langle \psi | \phi \rangle = \langle \hat{U}\psi | \hat{U}\phi \rangle$

■ Characteristics of Unitary Operator for Quantum Computing

- The probability remains unchanged under unitary operators
- Any quantum states preserve their initial states after two identical unitary operators

■ Example of Unitary Operator

- Hadamard gate: turns $|0\rangle$ or $|1\rangle$ into the superposition of $|0\rangle$ and $|1\rangle$
- Matrix representation of the Hadamard gate: $\hat{H} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$
- Proof: $\hat{H}^\dagger = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$ and $\hat{H}^\dagger \hat{H} = \frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \hat{I}$

Brief Review of Linear Algebra: (11) Hermitian Operators

■ Definition of Hermitian Operator

- A linear operator \hat{H} is Hermitian (also known as self-adjoint), if it is equal to its own adjoint: $\hat{H} = \hat{H}^\dagger$

■ Properties of Hermitian Operator

- Real eigenvalues: Hermitian operator \hat{H} has real (not complex) eigenvalues as

$$\hat{H}|\psi\rangle = \lambda|\psi\rangle, \text{ where } \lambda \text{ is the eigenvalue and real value}$$

- Orthogonal eigenvectors: Eigenvectors corresponding to different eigenvalues of an Hermitian operator are orthogonal

$$\hat{H}|\psi_1\rangle = \lambda_1|\psi_1\rangle \text{ and } \hat{H}|\psi_2\rangle = \lambda_2|\psi_2\rangle \rightarrow \langle\psi_1|\psi_2\rangle = 0, \text{ if } \lambda_1 \neq \lambda_2$$

- Diagonalization: Hermitian operator \hat{H} can be diagonalized by a unitary operator \hat{U} as

$$\hat{U}\hat{H}\hat{U}^\dagger = \text{diag}(\lambda_1, \lambda_2, \dots, \lambda_n) = \begin{pmatrix} \lambda_1 & \cdots & 0 \\ 0 & \ddots & 0 \\ \vdots & \cdots & \lambda_n \end{pmatrix}, \text{ where } \lambda_i \text{ are the eigenvalues of } \hat{H}$$

■ Characteristics of Hermitian Operator for Quantum Computing

- Hermitian operators represent **observable physical quantities**, such as position, momentum, and energy
- **Hamiltonian is one of the Hermitian operators**, since Hamiltonian represents the total energy of a quantum system

Brief Review of Linear Algebra: (12) Taylor Expansion of an Operator

■ Definition of Taylor Expansion of Operator

- Similar to the Taylor expansion of a function, operators can be also approximated by the Taylor expansion

■ Formula of Taylor Expansion

- For an operator \hat{A} , the exponential of the operator is

$$e^{\hat{A}} = \sum_{n=0}^{\infty} \frac{(\hat{A})^n}{n!} = \hat{A} + \frac{1}{2!} \hat{A}\hat{A} + \frac{1}{3!} \hat{A}\hat{A}\hat{A} + \dots$$

■ Characteristics of Taylor Expansion of Operator for Quantum Computing

- The time evolution of a quantum state is governed by the exponential of a time-independent Hamiltonian operator \hat{H} as

$$e^{-j\hat{H}t/\hbar} = \sum_{n=0}^{\infty} \frac{1}{n!} \left(-\frac{j\hat{H}t}{\hbar} \right)^n$$

where \hbar is the reduced Planck's constant and t is time

- Taylor expansion is used in perturbation theory to approximate the effects of small perturbations

Brief Review of Differential Equation: Ordinary Differential Equation (ODE)

■ Definition of ODE

- An equation involving a function of one independent variable and its derivatives
- The generalized expression of an ODE for the unknown function y is

$$\frac{d^n}{dx^n}y + a_{n-1}(x)\frac{d^{n-1}}{dx^{n-1}}y + \cdots + a_1(x)\frac{d}{dx}y + a_0(x)y = g(x)$$

where $a_i(x)$ and $g(x)$ are given functions

■ Properties of ODE

- Order: The highest derivative of the unknown function in the ODE
- Homogeneous ODE: If $g(x) = 0$ (otherwise, $g(x) \neq 0$, inhomogeneous ODE)

■ Mathematical Methods to Solve ODE

- Analytical methods: only some ODEs can be solved by exact analytical methods
- Numerical methods: most of ODEs are solved by numerical methods with approximations

Brief Review of Differential Equation: Partial Differential Equation (PDE)

■ Definition of partial Derivative

- Derivative of a function with respect to one of the independent variables, with the others being constant
- The partial derivative of a function y at the point $\mathbf{a} = (a_1, a_2, \dots, a_n)$ with respect to the i^{th} variable x_i is defined as

$$\frac{\partial}{\partial x_i} f(\mathbf{a}) = \lim_{h \rightarrow 0} \frac{f(a_1, \dots, a_i + h, \dots, a_n) - f(a_1, \dots, a_i, \dots, a_n)}{h}$$

■ Definition of PDE

- An equation involving a function of multiple independent variables and its partial derivatives
- The generalized expression of an ODE for the unknown function y with the independent variables x and t is

$$\frac{\partial^n}{\partial t^n} y + a_{n-1}(x, t) \frac{\partial^{n-1}}{\partial t^{n-1}} y + \dots + a_1(x, t) \frac{\partial}{\partial t} y + a_0(x, t) y = g(x, t)$$

where $a_i(x, t)$ and $g(x, t)$ are given functions

■ Example PDE in Quantum Computing

- Schrödinger equation: time evolution of a quantum system can be represented by a linear PDE in time variable

$$j\hbar \frac{d}{dt} |\psi\rangle = \hat{H} |\psi\rangle$$

NOTE: You don't have to solve Schrödinger equation by yourself.
There are various numerical tools to solve it.

Brief Review of Differential Equation: Green's Function

■ Definition of Green's Function

- Impulse response of an inhomogeneous linear differential operator \hat{L} with specified boundary conditions
- Green's function is often utilized to solve an inhomogeneous differential equation of $\hat{L}y(x) = f(x)$

■ Solving Inhomogeneous Differential Equation Using Green's Function

- For a given forcing term $f(x)$, the forcing term can be expressed with Dirac-delta function as

$$f(x) = \int_{\mathbb{R}^n} f(r) \delta(x - r) dr$$

Where Dirac-delta function is $\delta(x - r) \begin{cases} \infty, & \text{if } x = r \\ 0, & \text{if } x \neq r \end{cases}$ and satisfies $\int_{\mathbb{R}^n} \delta(r) dr = 1$

- For a given linear differential operator $\hat{L}(x)$, the Green's function $G(x)$ can be obtained from the following relation

$$\hat{L}G(x, r) = \delta(x - r)$$

NOTE: Most of Green's functions corresponding to the specific \hat{L} can be found in https://en.wikipedia.org/wiki/Green%27s_function

- Using the above relation, the inhomogeneous differential equation satisfies the following relations

$$f(r)\hat{L}G(x, r) = f(r)\delta(x - r) \longrightarrow \hat{L}f(r)G(x, r) = f(r)\delta(x - r)$$

- Thus, by integrating over the region \mathbb{R}^n , the unknown function $y(x)$ can be expressed as

$$\therefore y(x) = \int_{\mathbb{R}^n} f(r)G(x, r) dr$$

Brief Review of Vector Calculus: (1) Divergence Theorem

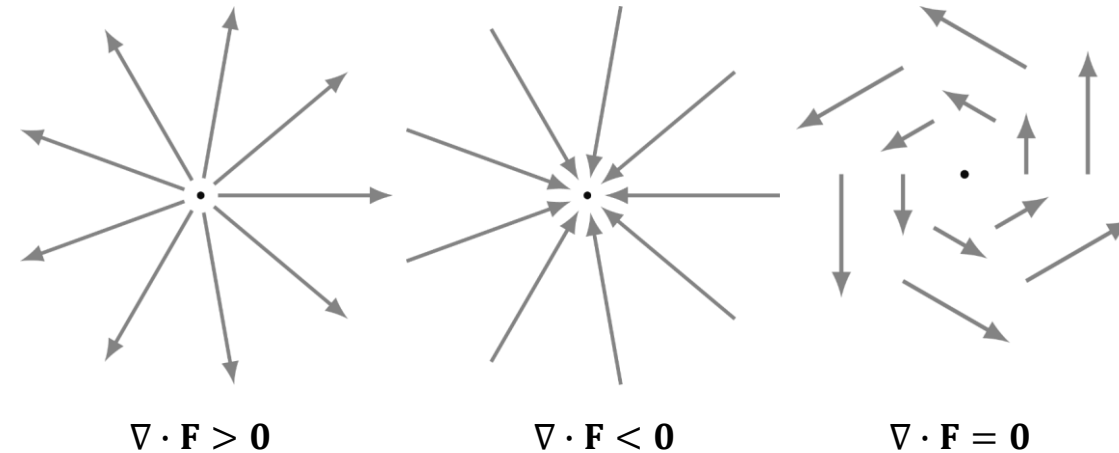
■ Definition of Divergence

- The divergence is the flux through the surface of a vector field \mathbf{F} , defined at $x = x_0$ as

$$\nabla \cdot \mathbf{F} \Big|_{x=x_0} = \lim_{V \rightarrow 0} \frac{1}{|V|} \oint_{\partial V} \mathbf{F} \cdot d\mathbf{a}$$

- For cartesian coordinate, the divergence of a vector field \mathbf{F} is

$$\nabla \cdot \mathbf{F} = \frac{\partial F_x}{\partial x} + \frac{\partial F_y}{\partial y} + \frac{\partial F_z}{\partial z}$$



■ Definition of Divergence Theorem (also Known as Gauss's Theorem)

- The surface integral of a vector field over a closed surface is equal to the volume integral of the divergence over the region enclosed by the surface

$$\int_V (\nabla \cdot \mathbf{F}) dV = \int_{\partial V} \mathbf{F} \cdot d\mathbf{a}$$

↑ Volume Integral ↑ Surface Integral

Brief Review of Vector Calculus: (2) Stokes' Theorem

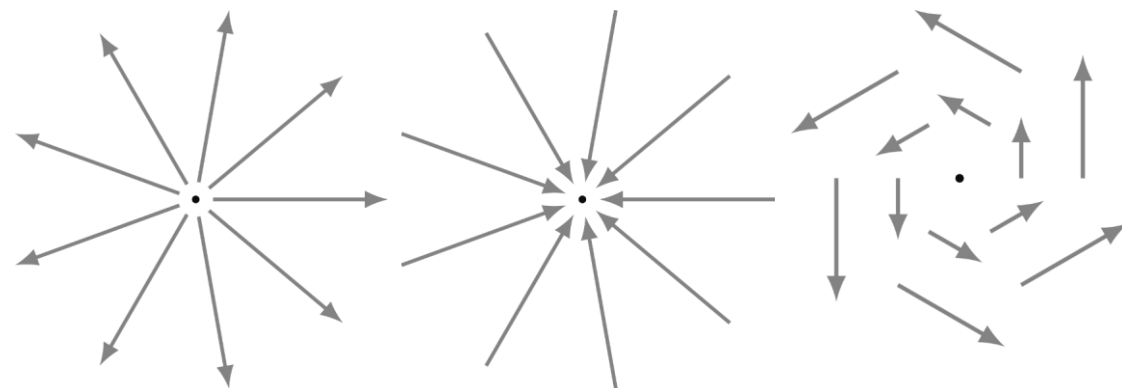
■ Definition of Curl

- The curl is the circulation of a vector field \mathbf{F} , defined at $\mathbf{x} = \mathbf{x}_0$ as

$$\nabla \times \mathbf{F} \Big|_{\mathbf{x}=\mathbf{x}_0} = \lim_{A \rightarrow 0} \frac{1}{|A|} \oint_{\partial A} \mathbf{F} \cdot d\mathbf{l}$$

- For cartesian coordinate, the curl of a vector field \mathbf{F} is

$$\nabla \times \mathbf{F} = \left(\frac{\partial F_z}{\partial y} - \frac{\partial F_y}{\partial z} \right) \hat{x} + \left(\frac{\partial F_x}{\partial z} - \frac{\partial F_z}{\partial x} \right) \hat{y} + \left(\frac{\partial F_y}{\partial x} - \frac{\partial F_x}{\partial y} \right) \hat{z}$$



$\nabla \times \mathbf{F} = \mathbf{0}$

$\nabla \times \mathbf{F} = \mathbf{0}$

$\nabla \times \mathbf{F} \neq \mathbf{0}$

Figure. Example visualizations of curl of \mathbf{F}

■ Definition of Stokes' Theorem

- The line integral of a vector field over a loop is equal to the surface integral of its curl over the enclosed surface

$$\int_A (\nabla \times \mathbf{F}) \cdot d\mathbf{a} = \oint_{\partial A} \mathbf{F} \cdot d\mathbf{l}$$



Surface Integral



Line Integral

Brief Review of Dimensional Analysis: Physical Unit Conversion

■ Definition of Physical Unit Conversion

- Analysis of the relationships between physical quantities by identifying their base quantities and units of measurement
- Using the international standard unit systems, intuitive analysis and comparison between variables are possible

■ Physical Unit Conversion in Quantum Computing

- In physics, particularly in superconducting quantum circuits, many variables have unfamiliar physical units
- Example: qubit energy in [Hz] or in [rad/s] by reducing the physical constants as 1

$$\begin{aligned}\text{qubit energy [J]} &= \hbar \times \text{qubit angular frequency [rad/s]} \\ &= h \times \text{qubit frequency [Hz]}\end{aligned}$$

Why?


In practice, we measure the qubit energy levels by RF spectroscopy in frequency units

■ Some Notable Physical Constants

- Planck's constant $h \approx 6.63 \times 10^{-34}$ [J·s]
- Charge of an electron $e \approx 1.60 \times 10^{-19}$ [C]
- Speed of light in vacuum $c \approx 3.00 \times 10^8$ [m/s]
- Impedance of vacuum $Z_\eta \approx 377$ [Ω]
- Boltzmann constant $k_B \approx 1.38 \times 10^{-23}$ [J/K]
- Vacuum permeability $\mu_0 \approx 1.26 \times 10^{-6}$ [H/m]
- Vacuum permittivity $\epsilon_0 \approx 8.85 \times 10^{-12}$ [F/m]
- Magnetic flux quantum $\Phi_0 = \frac{h}{2e} \approx 2.07 \times 10^{-15}$ [Wb]

See Also...

■ Textbooks:

- [1] Mary L. Boas, *Mathematical Methods in the Physical Sciences*, John Wiley & Sons, 2006.  * recommended
- [2] Erwin O. Kreyszig, *Advanced Engineering Mathematics*, John Wiley & Sons, 2011.
- [3] George B. Arfken, *Mathematical Methods for Physicists*, Elsevier, 2012.