

**REGIONAL DOCTORAL PROGRAM IN THEORETICAL AND
EXPERIMENTAL PARTICLE PHYSICS**

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**Exactly solvable models in quantum mechanics
and
their application in quantum computing**
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I ————— The exactly solvable models —————

1. Methods for obtaining exact and approximate solutions of the evolution of quantum-mechanical problems.

The cyclic evolution of quantum systems described by time-periodic Hamiltonians.

2 . Construction of a class of time-periodic Hamiltonians in the close analytical form.

Calculation of corresponding cyclic solution

II ————— Quantum computing —————

3. Construction of a universal set of gates for quantum computers used the exactly solvable time-dependent Hamiltonian.

A method for obtaining entanglement operators.

Construction of a Time-Dependent Hamiltonian

Let the state $\Psi(r, t)$ of a quantum system evolve according to the matrix Schrödinger equation

$$i \frac{d\Psi(r, t)}{dt} = H(r, t)\Psi(r, t), \quad (1)$$

where $H(r, t)$ is periodic in time t , $H(t + T) = H(t)$, and has the form

$$H(r, t) = \hat{p}_r^2 + V(r, t). \quad (2)$$

Here, the potential matrix $V(r, t)$ is a $d \times d$ time-periodic Hermitian matrix such that $V(r, t + T) = V(r, t)$ and $\hat{p}_r = -i\nabla_r$ is the angular momentum operator determining the kinetic energy.

In terms of the evolution operator $\mathcal{U}(t) \equiv \mathcal{U}(t, 0)$, $\mathcal{U}(0) = 1$, the solution of Eq. (1) is written as

$$\Psi(r, t) = \mathcal{U}(t)\Psi(r, 0), \quad (3)$$

where $\Psi(r, 0)$ is the initial state and $\mathcal{U}(t)$ satisfies the equation

$$i \frac{d\mathcal{U}(t)}{dt} = H(t)\mathcal{U}(t), \quad (4)$$

which relates $H(t)$ and $\mathcal{U}(t)$.

$$H(t + T) = H(t)$$

$$V(r, t + T) = V(r, t)$$

$$\hat{p}_r = -i\nabla_r$$

Construction of a Time-Dependent Hamiltonian

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$$i\frac{d\Psi(r,t)}{dt} = H(r,t)\Psi(r,t) \quad (1)$$

In addition to the evolution operator transforming the initial state vector $|\Psi(t=0)\rangle$ to the state vector $|\Psi(t)\rangle$ at an arbitrary instant, it is convenient to introduce the unitary transformation $[\mathcal{S}^\dagger(t) = \mathcal{S}^{-1}(t), \mathcal{S}^\dagger(t)\mathcal{S}(t) = 1]$ through the relation

$$\Psi(r,t) = \mathcal{S}(t)\tilde{\Psi}(r,t) \quad (5)$$

such that, in the equation

$$i\frac{d\tilde{\Psi}(t)}{dt} = \tilde{H}(r)\tilde{\Psi}(t) \quad (6)$$

following from Eq. (1) with substitution (5), the Hamiltonian

$$\tilde{H} = \mathcal{S}^\dagger(t)H(t)\mathcal{S}(t) - i\mathcal{S}^\dagger(t)(d/dt)\mathcal{S}(t) \quad (7)$$

is time independent; i.e., $d\tilde{H}/dt = 0$.

The condition (7) provides the equation for $\mathcal{S}(t)$,

$$\dot{\mathcal{S}}^\dagger H \mathcal{S} + \mathcal{S}^\dagger (\partial H / \partial t) \mathcal{S} + \mathcal{S}^\dagger H \dot{\mathcal{S}} - i\hbar \dot{\mathcal{S}}^\dagger \dot{\mathcal{S}} - i\hbar \mathcal{S}^\dagger \ddot{\mathcal{S}} = 0 \quad (8)$$

where $\dot{\mathcal{S}} = (d/dt)\mathcal{S}$.

The solution of Eq. (6) for new functions $\tilde{\Psi}(r,t) = \mathcal{S}^\dagger(t)\Psi(r,t)$ has the form

$$\tilde{\Psi}(r,t) = \exp(-i\tilde{H}(r)t)\tilde{\Psi}(r,0) \quad (9)$$

and is determined by the solution of the time-independent problem

$$\tilde{H}|F(\tilde{\mathcal{E}})\rangle = \tilde{\mathcal{E}}|F(\tilde{\mathcal{E}})\rangle. \quad (10)$$

Eqs. (6) and (9)



$$\Psi(r,t) = \mathcal{S}(t)\exp(-i\tilde{H}(r)t)\tilde{\Psi}(r,0) \quad (11)$$

Beginning with the time-independent equation

$$\tilde{H}|F(\tilde{\mathcal{E}})\rangle = \tilde{\mathcal{E}}|F(\tilde{\mathcal{E}})\rangle \quad \longleftarrow \quad \text{Eq. (10)}$$

whose solution is known numerically or analytically, specifying the transformation $\mathcal{S}(t)$ in the explicit form and using equation

$$\tilde{H} = \mathcal{S}^\dagger(t)H(t)\mathcal{S}(t) - i\mathcal{S}^\dagger(t)(d/dt)\mathcal{S}(t) \quad \longleftarrow \quad \text{Eq. (7)}$$

and the unitarity of $\mathcal{S}(t)$ one can determine the time-dependent Hamiltonians

$$H(t) = \mathcal{S}(t)\tilde{H}\mathcal{S}^\dagger(t) + i\dot{\mathcal{S}}(t)\mathcal{S}^\dagger(t) \quad (12)$$

and solutions of Schrödinger equation

$$i\frac{d\Psi(r, t)}{dt} = H(r, t)\Psi(r, t) \quad \longleftarrow \quad \text{Eq. (1)}$$

by formula

$$\Psi(r, t) = \mathcal{S}(t)\exp(-i\tilde{H}(r)t)\tilde{\Psi}(r, 0) \quad \longleftarrow \quad \text{Eq. (11)}$$

Expression

$$H(t) = \mathcal{S}(t)\tilde{H}\mathcal{S}^\dagger(t) + i\dot{\mathcal{S}}(t)\mathcal{S}^\dagger(t)$$

immediately provides the relation between the Hamiltonian at $t = 0$ and time-independent Hamiltonian \tilde{H} :

$$H(0) = \mathcal{S}(0)\tilde{H}\mathcal{S}^\dagger(0) + i\dot{\mathcal{S}}(0)\mathcal{S}^\dagger(0).$$

$$\Psi(r, t) = \mathcal{U}(t)\Psi(r, 0) \quad (3)$$

$$\Psi(r, t) = \mathcal{S}(t)\tilde{\Psi}(r, t) \quad (5) \quad \Psi(r, t) = \mathcal{S}(t)\exp(-i\tilde{H}(r)t)\tilde{\Psi}(r, 0) \quad (11)$$



Comparison of Eqs. (3), (5), and (11) provides the important relation between $\mathcal{U}(t)$ and $\mathcal{S}(t)$,

$$\mathcal{U}(t) = \mathcal{S}(t)\exp(-i\tilde{H}t)\mathcal{S}^\dagger(0).$$

Construction of a 2×2 Periodic Potential Matrix

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We investigate the systems of two coupled Schrödinger equations with the Hamiltonian

$$H(r, t) = h(r) + h_1(r, t). \quad (1)$$

Here, $h(r)$ is the time-independent part of the Hamiltonian, the Hamiltonian $h_1(r, t)$ is a periodic function of time, and $h_1(r, t + T) = h_1(r, t)$ and can be represented in the form

$$h_1(r, t) = \sum_i \hat{\sigma}_i B_i(r, t), \quad (2)$$

where $\hat{\sigma}_i$ are the Pauli matrices and $B_i(r, t)$ are periodic in time.

Our aim is to construct families of time-dependent Hamiltonians $H(r, t)$ of form (1) for which exact solutions of Schrodinger equation can be found.

Consider the time-independent Hamiltonian

$$\tilde{H}(r) = p_r^2 + V(r), \quad (3)$$

where $V(r)$ is the 2×2 real symmetric potential matrix, and the time-dependent unitary transformation matrix $\mathcal{S}(t)$ that transforms known time-independent Hamiltonian

to time-dependent Hamiltonian

$$H(t) = \mathcal{S}(t)\tilde{H}\mathcal{S}^\dagger(t) + i\dot{\mathcal{S}}(t)\mathcal{S}^\dagger(t) \quad (4)$$

Construction of a 2×2 Periodic Potential Matrix

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Consider the transformation $\mathcal{S}(t)$ in the form of the 2×2 matrix

$$\mathcal{S}(t) = \exp(-is \cdot \mathbf{q}(t)) = \exp\left(-i \sum_{i=1}^3 s_i q_i(t)\right), \quad (5)$$

where $\mathbf{s} = \boldsymbol{\sigma}/2$ is the spin operator, $\boldsymbol{\sigma} = (\hat{\sigma}_1, \hat{\sigma}_2, \hat{\sigma}_3)$, $\hat{\sigma}_i$ are the Pauli matrices, and q_i are arbitrary real functions of time.

$$\begin{array}{ccc} i \frac{d\Psi(r, t)}{dt} = H(r, t)\Psi(r, t) & & H(t) = \mathcal{S}(t)\tilde{H}\mathcal{S}^\dagger(t) + i\dot{\mathcal{S}}(t)\mathcal{S}^\dagger(t) \\ \downarrow & & \\ \tilde{H}(r) = p_r^2 + V(r) & \xrightarrow{\mathcal{S}(t)} & H(r, t) = p_r^2 + \exp(-is \cdot \mathbf{q}(t))V(r) \\ & & \times \exp(is \cdot \mathbf{q}(t)) + \mathbf{s} \cdot \dot{\mathbf{q}}(t). \\ & & \swarrow \\ & & |\Psi(r, t)\rangle = \exp(-is \cdot \mathbf{q}(t)) \\ & & \times \exp(-i\tilde{H}(r)t)|\tilde{\Psi}(r, t=0)\rangle. \end{array}$$

Construction of a 2×2 Periodic Potential Matrix

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It is convenient to represent 2×2 Hamiltonian

$$\tilde{H}(r) = p_r^2 + V(r)$$

as the sum of the diagonal and traceless matrices:

$$\begin{aligned}\tilde{H}(r) &= p_r^2 \hat{I} + \begin{pmatrix} v_{11}(r) & v_{12}(r) \\ v_{21}(r) & v_{22}(r) \end{pmatrix} \\ &= \left(p_r^2 + \frac{v_{11}(r) + v_{22}(r)}{2} \right) \hat{I} + \begin{pmatrix} \frac{v_{11}(r) - v_{22}(r)}{2} & v_{12}(r) \\ v_{21}(r) & -\frac{v_{11}(r) - v_{22}(r)}{2} \end{pmatrix} \\ &= (p_r^2 + u(r)) \hat{I} + \boldsymbol{\sigma} \cdot \mathbf{B}(r),\end{aligned}$$

where v_{ij} are real, $v_{12} = v_{21}$, $u = (v_{11} + v_{22})/2$, $B_1 = v_{12}$, $B_2 = 0$, $B_3 = (v_{11} - v_{22})/2$, and \hat{I} is the identity matrix.

If $\Psi(r, 0) = \tilde{\psi}(r, 0) \implies$ then $\mathcal{S}(0) = 1$.

$$\mathcal{U}(t) = \mathcal{S}(t) \exp(-i\tilde{H}t) \mathcal{S}^\dagger(0)$$

$$\mathcal{S}(t) = \exp(-is \cdot \mathbf{q}(t)) = \exp\left(-i \sum_{i=1}^3 s_i q_i(t)\right)$$

$$\mathcal{U}(t) = \mathcal{S}(t) \exp(-i\tilde{H}t) = \exp(is \cdot \mathbf{q}(t)) \exp(-i\tilde{H}t).$$

The evolution operator after the period is written as

$$\mathcal{U}(T) = \exp(-is \cdot \mathbf{q}(T)) \exp(-i\tilde{H}T).$$

Particular cases

SU(2) transformations

$\mathbf{q}(t)$ are linear functions of time: $q_i(t) = \omega_i t$.

1

$$\mathcal{P}_3(t) = \exp(-i\hat{\sigma}_3\omega t/2) = \begin{pmatrix} \exp(-i\omega t/2) & 0 \\ 0 & \exp(i\omega t/2) \end{pmatrix},$$

Particular cases

where ω is the angular frequency.

$$H(r, t) = (p_r^2 + u(r))\hat{I}$$

$$+ \begin{pmatrix} \frac{v_{11}(r) - v_{22}(r) + \omega}{2} & v_{12}(r)\exp(-i\omega t) \\ v_{21}(r)\exp(i\omega t) & -\frac{v_{11}(r) - v_{22}(r) + \omega}{2} \end{pmatrix} \leftrightarrow \tilde{H}(r) = (p_r^2 + u(r))\hat{I} + \tilde{\Omega}(r) \begin{pmatrix} \cos\tilde{\theta}(r) & \sin\tilde{\theta}(r) \\ \sin\tilde{\theta}(r) & -\cos\tilde{\theta}(r) \end{pmatrix}.$$

Here, $u(r) = (v_{11}(r) + v_{22}(r))/2$ can be treated as an analogue of the constant electric field, and the analogue of the magnetic field $\tilde{\mathbf{B}}(r)$ can be expressed in terms of the potential matrix as

$$\tilde{\mathbf{B}}(r) = \tilde{\Omega}(r)(\sin\tilde{\theta}(r), 0, \cos\tilde{\theta}(r)),$$

$$\begin{aligned} \tilde{\Omega}(r) &= (1/2)\sqrt{(v_{11}(r) - v_{22}(r))^2 + 4v_{12}(r)^2} \\ &= \sqrt{B_3^2(r) + B_1^2(r)}, \end{aligned}$$

where

$$\sin\tilde{\theta}(r) = \frac{v_{12}(r)}{\tilde{\Omega}(r)},$$

$$\cos\tilde{\theta}(r) = \frac{v_{11}(r) - v_{22}(r)}{2\tilde{\Omega}(r)}.$$

1

$$H(t, r) = (p_r^2 + u(r))\hat{I}$$

$$+ \Omega(r) \begin{pmatrix} \cos\theta(r) & \sin\theta(r) \exp(-i\omega t) \\ \sin\theta(r) \exp(i\omega t) & -\cos\theta(r) \end{pmatrix}$$

$$|\Psi_1(t)\rangle = \begin{pmatrix} \exp[-(i\omega t/2) - i\tilde{\mathcal{E}}_1 t] \cos(\tilde{\theta}/2) \\ \exp[(i\omega t/2) - i\tilde{\mathcal{E}}_1 t] \sin(\tilde{\theta}/2) \end{pmatrix},$$

$$|\Psi_2(t)\rangle = \begin{pmatrix} -\exp[-(i\omega t/2) - i\tilde{\mathcal{E}}_2 t] \sin(\tilde{\theta}/2) \\ \exp[(i\omega t/2) - i\tilde{\mathcal{E}}_2 t] \cos(\tilde{\theta}/2) \end{pmatrix}.$$

$$|\Phi_1\rangle = \begin{pmatrix} \cos(\tilde{\theta}/2) \\ \sin(\tilde{\theta}/2) \end{pmatrix}, \quad |\Phi_2\rangle = \begin{pmatrix} -\sin(\tilde{\theta}/2) \\ \cos(\tilde{\theta}/2) \end{pmatrix}$$

$$\tilde{\mathcal{E}}_1 = +\tilde{\Omega}, \quad \tilde{\mathcal{E}}_2 = -\tilde{\Omega}.$$

$$H(t) = \boldsymbol{\sigma} \cdot \mathbf{B}(t)$$

$$= \Omega \begin{pmatrix} \cos\theta & \sin\theta \exp(-i\omega t) \\ \sin\theta \exp(i\omega t) & -\cos\theta \end{pmatrix},$$

where

$$\mathbf{B}(t) = \Omega(\sin\theta \cos(\omega t), \sin\theta \sin(\omega t), \cos\theta)$$

$$\tilde{H} = \boldsymbol{\sigma} \cdot \tilde{\mathbf{B}} = \tilde{\Omega} \begin{pmatrix} \cos\tilde{\theta} & \sin\tilde{\theta} \\ \sin\tilde{\theta} & -\cos\tilde{\theta} \end{pmatrix}$$

with the spatially uniform magnetic field

$$\tilde{\mathbf{B}} = \tilde{\Omega}(\sin\tilde{\theta}, 0, \cos\tilde{\theta}).$$

2

Particular cases

$$\mathcal{G}_2(t) = \exp(-i\hat{\sigma}_2\omega_2 t/2) = \begin{pmatrix} \cos(\omega_2 t/2) & -\sin(\omega_2 t/2) \\ \sin(\omega_2 t/2) & \cos(\omega_2 t/2) \end{pmatrix}$$

$$H(r, t) = (p_r^2 + u(r))\hat{I}$$

$$+ \begin{pmatrix} \frac{v_{11} - v_{22}}{2} \cos \omega_2 t - v_{12} \sin \omega_2 t & v_{12} \cos \omega_2 t + \frac{v_{11} - v_{22}}{2} \sin \omega_2 t - i\omega_2/2 \\ v_{12} \cos \omega_2 t + \frac{v_{11} - v_{22}}{2} \sin \omega_2 t + i\omega_2/2 & -\left(\frac{v_{11} - v_{22}}{2} \cos \omega_2 t - v_{12} \sin \omega_2 t\right) \end{pmatrix}.$$

$$|\Psi_1(t)\rangle = \begin{pmatrix} \cos(\omega_2 t/2) \exp(-i\tilde{\mathcal{E}}_1 t) \cos \tilde{\theta}/2 - \sin(\omega_2 t/2) \exp(-i\tilde{\mathcal{E}}_2 t) \sin \tilde{\theta}/2 \\ \sin(\omega_2 t/2) \exp(-i\tilde{\mathcal{E}}_1 t) \cos \tilde{\theta}/2 + \cos(\omega_2 t/2) \exp(-i\tilde{\mathcal{E}}_2 t) \sin \tilde{\theta}/2 \end{pmatrix},$$

$$|\Psi_2(t)\rangle = \begin{pmatrix} -\cos(\omega_2 t/2) \exp(-i\tilde{\mathcal{E}}_1 t) \sin \tilde{\theta}/2 - \sin(\omega_2 t/2) \exp(-i\tilde{\mathcal{E}}_2 t) \cos \tilde{\theta}/2 \\ -\sin(\omega_2 t/2) \exp(-i\tilde{\mathcal{E}}_1 t) \sin \tilde{\theta}/2 + \cos(\omega_2 t/2) \exp(-i\tilde{\mathcal{E}}_2 t) \cos \tilde{\theta}/2 \end{pmatrix}.$$

Particular cases

3

$$\mathcal{G}_1(t) = \exp(-i\hat{\sigma}_1\omega_1 t/2) = \begin{pmatrix} \cos(\omega_1 t/2) & -i \sin(\omega_1 t/2) \\ -i \sin(\omega_1 t/2) & \cos(\omega_1 t/2) \end{pmatrix}.$$

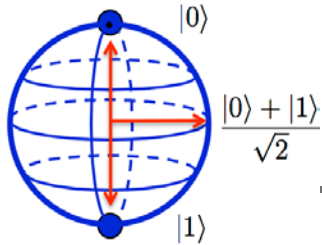
$$H(r, t) = (p_r^2 + u(r))\hat{I} + \begin{pmatrix} \frac{V_{11} - V_{22}}{2} \cos(\omega_1 t) & V_{12} - \frac{\omega_1}{2} + i \frac{V_{11} - V_{22}}{2} \sin(\omega_1 t) \\ V_{12} - \frac{\omega_1}{2} - i \frac{V_{11} - V_{22}}{2} \sin(\omega_1 t) & -\frac{V_{11} - V_{22}}{2} \cos(\omega_1 t) \end{pmatrix}.$$

$$|\Psi_1(t)\rangle = \begin{pmatrix} \cos(\omega_1 t/2) \exp(-i\tilde{\mathcal{E}}_1 t) \cos\tilde{\theta}/2 - i \sin(\omega_1 t/2) \exp(-i\tilde{\mathcal{E}}_2 t) \sin\tilde{\theta}/2 \\ -i \sin(\omega_1 t/2) \exp(-i\tilde{\mathcal{E}}_1 t) \cos\tilde{\theta}/2 + \cos(\omega_1 t/2) \exp(-i\tilde{\mathcal{E}}_2 t) \sin\tilde{\theta}/2 \end{pmatrix},$$

$$|\Psi_2(t)\rangle = \begin{pmatrix} -\cos(\omega_1 t/2) \exp(-i\tilde{\mathcal{E}}_1 t) \sin\tilde{\theta}/2 - i \sin(\omega_1 t/2) \exp(-i\tilde{\mathcal{E}}_2 t) \cos\tilde{\theta}/2 \\ i \sin(\omega_1 t/2) \exp(-i\tilde{\mathcal{E}}_1 t) \sin\tilde{\theta}/2 + \cos(\omega_1 t/2) \exp(-i\tilde{\mathcal{E}}_2 t) \cos\tilde{\theta}/2 \end{pmatrix}.$$

● 0

● 1

**Qubit**

The classical bit is a system having two values, 0 and 1. Any quantum system having at least two states can be taken as the qubit. One state is denoted as $|0\rangle$, and the other state, orthogonal to the first, is denoted as $|1\rangle$. An arbitrary state of the qubit can be represented as

$$|\phi\rangle = a|0\rangle + b|1\rangle, \quad |a|^2 + |b|^2 = 1$$

where a and b are complex numbers. The components of two-dimensional vectors $|0\rangle$, $|1\rangle$, and $|\phi\rangle$ are written in the form of the columns

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad |\phi\rangle = a \begin{pmatrix} 1 \\ 0 \end{pmatrix} + b \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} a \\ b \end{pmatrix}.$$

A convenient example of the qubit is the nuclear or electron spin $s = \frac{1}{2}\boldsymbol{\sigma}$.

This spin in the constant external magnetic field has two energy levels corresponding to the spin directions along and against the field.

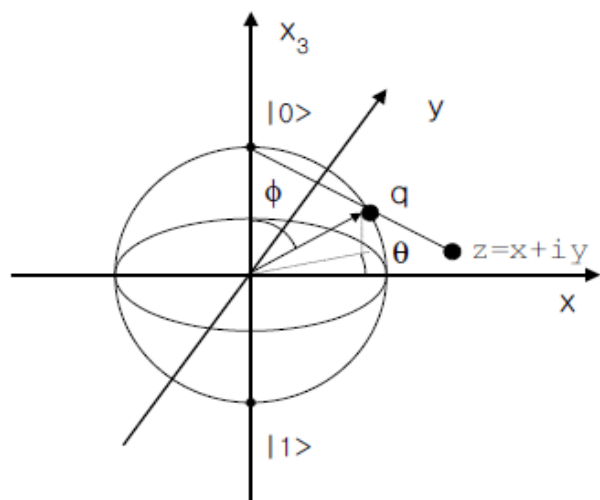
In this case, the Hamiltonian has the form $\tilde{H} = \boldsymbol{\sigma} \cdot \tilde{\mathbf{B}} = \tilde{\Omega} \begin{pmatrix} \cos \tilde{\theta} & \sin \tilde{\theta} \\ \sin \tilde{\theta} & -\cos \tilde{\theta} \end{pmatrix}$

$$|\phi_1\rangle = \begin{pmatrix} \cos(\tilde{\theta}/2) \\ \sin(\tilde{\theta}/2) \end{pmatrix} = \cos(\tilde{\theta}/2)|0\rangle + \sin(\tilde{\theta}/2)|1\rangle, \quad |\phi_2\rangle = \begin{pmatrix} -\sin(\tilde{\theta}/2) \\ \cos(\tilde{\theta}/2) \end{pmatrix} = -\sin(\tilde{\theta}/2)|0\rangle + \cos(\tilde{\theta}/2)|1\rangle.$$

Here, $a = \cos(\tilde{\theta}/2)$ and $b = \sin(\tilde{\theta}/2)$

$\longleftarrow |\phi_1\rangle$

$|\phi_2\rangle \longrightarrow a = -\sin(\tilde{\theta}/2)$ and $b = \cos(\tilde{\theta}/2)$





The vector $|\phi\rangle = \begin{pmatrix} a \\ b \end{pmatrix}$ is transformed to the vector $|\phi'\rangle = \begin{pmatrix} a' \\ b' \end{pmatrix}$ by means of the second-order unitary matrix ${}^{\mathcal{U}}$

$$|\phi'\rangle = {}^{\mathcal{U}}(2 \times 2)|\phi\rangle.$$

One - qubit quantum gate $\mathbb{C}^2 \rightarrow \mathbb{C}^2$

Two-qubit quantum gate $\mathbb{C}^2 \otimes \mathbb{C}^2 \rightarrow \mathbb{C}^2 \otimes \mathbb{C}^2$

Main conditions necessary for constructing the quantum computer is the existence of a universal set of one- and two-qubit quantum gates that can provide an arbitrary unitary transformation $\mathcal{U}(t)$ of an n -qubit quantum system (register) in the $N = 2^n$ - dim Hilbert space $\mathcal{H} = \mathcal{H}_1 \otimes \dots \otimes \mathcal{H}_n$, where $\mathcal{H}_j \cong \mathbb{C}^2$. The basis consisting of 2^n vectors is taken in the form

$$|j_0\rangle = |0\rangle \otimes |0\rangle \dots \otimes |0\rangle$$

$$|j_1\rangle = |0\rangle \otimes |0\rangle \dots \otimes |1\rangle$$

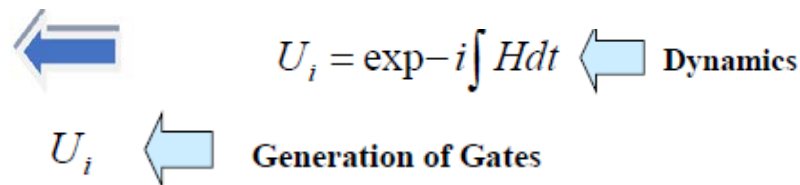
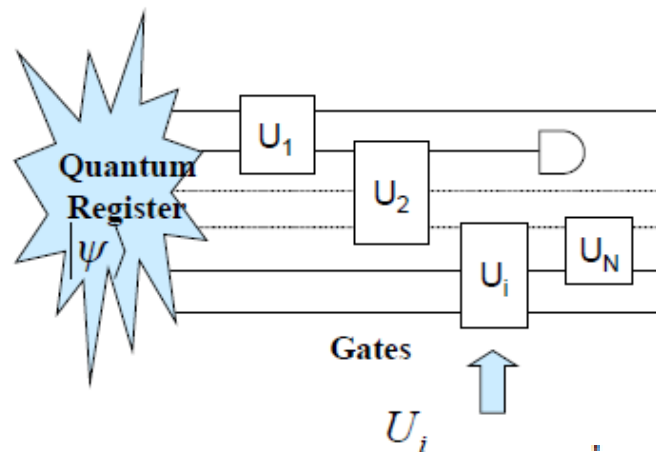
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$$|j_{2^n-1}\rangle = |1\rangle \otimes |1\rangle \dots \otimes |1\rangle.$$

$$|i_1, i_2, \dots, i_n\rangle = |i_1\rangle \otimes \dots \otimes |i_n\rangle \equiv |j\rangle, \quad i_1, i_2, \dots, i_n = \{0, 1\} \quad \Rightarrow \quad |\Psi\rangle = \sum_{k=0}^{2^n-1} a_k |j_k\rangle.$$

a_i are the projections of the $|\Psi\rangle$ vector on the unit vectors $|j_0\rangle, |j_1\rangle, \dots, |j_{2^n-1}\rangle$, and $\sum_k a_k^2 = 1$.

Quantum Computation



The computation process on the quantum computer is considered as the transformation of the initial state vector $|\Psi_0\rangle$ to the final vector $|\Psi_f\rangle$ by means of the $2^n \times 2^n$ unitary evolution matrix ${}^{\mathcal{O}}\mathcal{U}(t)$:

$$|\Psi_f\rangle = {}^{\mathcal{O}}\mathcal{U}(2^n \times 2^n)|\Psi_0\rangle.$$

It is convenient to take an initial state such that all its qubits are in the $|0\rangle$ state: $|\Psi_0\rangle = |0_1\rangle \otimes |0_2\rangle \dots \otimes |0_n\rangle = |0_1, 0_2, \dots, 0_n\rangle \equiv |j_0\rangle$. This operation is called preparation or initialization of the quantum register. The matrices ${}^{\mathcal{O}}\mathcal{U}(2^n \times 2^n)$ determine the dynamic evolution of the quantum system. The algorithm of solving the problem is specified by the ${}^{\mathcal{O}}\mathcal{U}(2^n \times 2^n)$ transformation matrix, which ensures the quantum computation process at each given instant.

The possibility of the decomposition of the $\mathcal{U}(2^n \times 2^n)$ matrix in the ordered product of the second- and fourth-order matrices is usually considered:

$$\mathcal{U}(2^n \times 2^n) = \prod_{i,j} \mathcal{U}_i(2 \times 2) \otimes \mathcal{U}_j(2^2 \times 2^2).$$

The second-order matrices $\mathcal{U}_i(2 \times 2)$ transform the state vectors of one qubit:

$$\begin{pmatrix} a' \\ b' \end{pmatrix}_i = \begin{pmatrix} u_{11} & u_{12} \\ u_{21} & u_{22} \end{pmatrix}_i \begin{pmatrix} a \\ b \end{pmatrix}_i.$$

The fourth-order matrices $\mathcal{U}_j(2^2 \times 2^2)$ transform the state vectors of pairs of qubits.

Consider the quantum system that evolves according to Schrödinger equation

$$i \frac{d\Psi(r, t)}{dt} = H(r, t)\Psi(r, t)$$

with Hamiltonian

$$H(t) = \lambda \begin{pmatrix} \cos \tilde{\theta} \cos(\omega_1 t) & \sin \tilde{\theta} - \omega_1/2\lambda + i \cos \tilde{\theta} \sin(\omega_1 t) \\ \sin \tilde{\theta} - \omega_1/2\lambda - i \cos \tilde{\theta} \sin(\omega_1 t) & -\cos \tilde{\theta} \cos(\omega_1 t) \end{pmatrix}$$

This Hamiltonian and corresponding cyclic solutions

$$|\Psi_1(t)\rangle = \begin{pmatrix} \cos(\omega_1 t/2) \exp(-i\tilde{\mathcal{E}}_1 t) \cos \tilde{\theta}/2 - i \sin(\omega_1 t/2) \exp(-i\tilde{\mathcal{E}}_2 t) \sin \tilde{\theta}/2 \\ -i \sin(\omega_1 t/2) \exp(-i\tilde{\mathcal{E}}_1 t) \cos \tilde{\theta}/2 + \cos(\omega_1 t/2) \exp(-i\tilde{\mathcal{E}}_2 t) \sin \tilde{\theta}/2 \end{pmatrix},$$

$$|\Psi_2(t)\rangle = \begin{pmatrix} -\cos(\omega_1 t/2) \exp(-i\tilde{\mathcal{E}}_1 t) \sin \tilde{\theta}/2 - i \sin(\omega_1 t/2) \exp(-i\tilde{\mathcal{E}}_2 t) \cos \tilde{\theta}/2 \\ i \sin(\omega_1 t/2) \exp(-i\tilde{\mathcal{E}}_1 t) \sin \tilde{\theta}/2 + \cos(\omega_1 t/2) \exp(-i\tilde{\mathcal{E}}_2 t) \cos \tilde{\theta}/2 \end{pmatrix}$$

are obtained by means of the transformation

$$\mathcal{G}(t) = \exp(-i\sigma_1 \omega_1 t/2)$$

of time-independent Hamiltonian

$$\tilde{H} = \boldsymbol{\sigma} \cdot \tilde{\mathbf{B}} = \tilde{\Omega} \begin{pmatrix} \cos \tilde{\theta} & \sin \tilde{\theta} \\ \sin \tilde{\theta} & -\cos \tilde{\theta} \end{pmatrix}$$

The initial qubit state is taken as one of the States

$$\phi_1 = \cos\tilde{\theta}/2|0\rangle + \sin\theta/2|1\rangle \quad \text{or} \quad \phi_2 = -\sin\theta/2|0\rangle + \cos\tilde{\theta}/2|1\rangle$$

of Hamiltonian

$$\tilde{H} = \boldsymbol{\sigma} \cdot \tilde{\mathbf{B}} = \tilde{\Omega} \begin{pmatrix} \cos\tilde{\theta} & \sin\tilde{\theta} \\ \sin\tilde{\theta} & -\cos\tilde{\theta} \end{pmatrix}$$

The evolution matrix corresponding to Hamiltonian

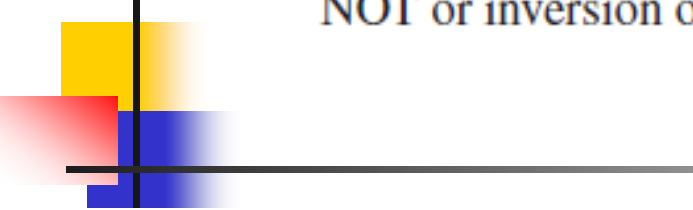
$$H(t) = \lambda \begin{pmatrix} \cos\tilde{\theta}\cos(\omega_1 t) & \sin\tilde{\theta} - \omega_1/2\lambda + i\cos\tilde{\theta}\sin(\omega_1 t) \\ \sin\tilde{\theta} - \omega_1/2\lambda - i\cos\tilde{\theta}\sin(\omega_1 t) & -\cos\tilde{\theta}\cos(\omega_1 t) \end{pmatrix}$$

has the form

$$\mathcal{U}_1(t) = \begin{pmatrix} \cos(\omega_1 t/2) & -i\sin(\omega_1 t/2) \\ -i\sin(\omega_1 t/2) & \cos(\omega_1 t/2) \end{pmatrix} \begin{pmatrix} \exp(-i\lambda t) & 0 \\ 0 & \exp(i\lambda t) \end{pmatrix}.$$

This evolution matrix provides a continuous set of single-qubit gates, which is specified by the parameters ω_1 and λ .

An important single-qubit transformation is the NOT or inversion operation


$$\text{NOT} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \sigma_x.$$

The NOT gate can be obtained from $\mathcal{U}_1(t)$ multiplied by i at

$$\omega_1 t = \pi \text{ and } \lambda t = 2n\pi: \quad \text{NOT} = iU_1(\omega_1 t = \pi, \lambda t = 2n\pi) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

Another special single-qubit gate can be obtained from $\mathcal{U}_1(t)$ by setting

$\omega_1 t = \pi$ and $\lambda t = \frac{\pi}{2}$ and multiplying the result by i :

$$Y = iU_1(\omega_1 t = \pi, \lambda t = \pi/2) = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \sigma_y.$$

The Z gate is obtained from $\mathcal{U}_1(t)$ for $\omega_1 t = 4\pi$ and $\lambda t = \frac{\pi}{2}$ after the multiplication by i :

$$Z = iU_1(\omega_1 t = 4\pi, \lambda t = \pi/2) = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \sigma_z.$$

$$\mathcal{U}_1(t) = \begin{pmatrix} \cos(\omega_1 t/2) & -i \sin(\omega_1 t/2) \\ -i \sin(\omega_1 t/2) & \cos(\omega_1 t/2) \end{pmatrix} \begin{pmatrix} \exp(-i\lambda t) & 0 \\ 0 & \exp(i\lambda t) \end{pmatrix}.$$

In quantum informatics, the Hadamard transform matrix

$$H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} = \frac{1}{\sqrt{2}} (\sigma_x + \sigma_z) \quad \text{is often used.}$$

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

$$H|1\rangle = H \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}} (|0\rangle - |1\rangle).$$

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

In this case, the evolution matrix $\mathcal{U}(t)$ corresponding to Hamiltonian $H(t)$ is

written as
$$\mathcal{U}(t) = \exp(-i\sigma_x \omega_1 t/2) \exp(-i\sigma_z \lambda t) \exp(-i\sigma_y \tilde{\theta}/2)$$

$$= \begin{pmatrix} \cos(\omega_1 t/2) & -i \sin(\omega_1 t/2) \\ -i \sin(\omega_1 t/2) & \cos(\omega_1 t/2) \end{pmatrix} \begin{pmatrix} \exp(-i\lambda t) & 0 \\ 0 & \exp(i\lambda t) \end{pmatrix} \begin{pmatrix} \cos(\tilde{\theta}/2) & -\sin(\tilde{\theta}/2) \\ \sin(\tilde{\theta}/2) & \cos(\tilde{\theta}/2) \end{pmatrix}.$$

$\mathcal{U}(t)$ for $t = 0$, $\tilde{\theta} = \frac{\pi}{2}$ and any ω_1 and λ values provides the gate

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \times \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} \Downarrow \quad \mathcal{U}(\omega_1, \lambda; t = 0, \tilde{\theta} = \pi/2) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}.$$

$$H = iU(\pi, 2\pi n, \tilde{\theta} = 0)U(\omega_1, \lambda, \tilde{\theta} = \pi/2; t = 0).$$

$$H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} = \frac{1}{\sqrt{2}} (\sigma_x + \sigma_z)$$

Hadamard gate H is obtained as the sequence of two transformations. The H gate applied to n qubits $|0\rangle$ generates the superposition of 2^n possible states and thus provides the binary representation of numbers from 0 to $2^n - 1$:

$$\begin{aligned} & (H \otimes H \otimes \dots \otimes H) |00\dots 0\rangle \\ &= \frac{1}{\sqrt{2^n}} ((|0\rangle + |1\rangle) \otimes (|0\rangle + |1\rangle) \otimes \dots \otimes (|0\rangle + |1\rangle)) = \frac{1}{\sqrt{2^n}} \sum_{k=0}^{2^n-1} |j_k\rangle. \end{aligned}$$

$\mathcal{U}(t)$ generates all $SU(2)$ matrices.

$$\begin{aligned} \mathcal{U}(t) &= \exp(-i\sigma_x \omega_1 t/2) \exp(-i\sigma_z \lambda t) \exp(-i\sigma_y \tilde{\theta}/2) \\ &= \begin{pmatrix} \cos(\omega_1 t/2) & -i \sin(\omega_1 t/2) \\ -i \sin(\omega_1 t/2) & \cos(\omega_1 t/2) \end{pmatrix} \begin{pmatrix} \exp(-i\lambda t) & 0 \\ 0 & \exp(i\lambda t) \end{pmatrix} \begin{pmatrix} \cos(\tilde{\theta}/2) & -\sin(\tilde{\theta}/2) \\ \sin(\tilde{\theta}/2) & \cos(\tilde{\theta}/2) \end{pmatrix}. \end{aligned}$$

$$\mathcal{U}(2^n \times 2^n) = \prod_{i,j} \mathcal{U}_i(2 \times 2) \otimes \mathcal{U}_j(2^2 \times 2^2).$$

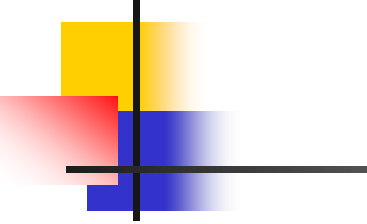
$$|00\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad |01\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, \quad |10\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \quad |11\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}.$$

$$\{|00\rangle = |0\rangle \otimes |0\rangle, |01\rangle = |0\rangle \otimes |1\rangle, \quad |10\rangle = |1\rangle \otimes |0\rangle, |11\rangle = |1\rangle \otimes |1\rangle\}:$$

$$|\Psi\rangle = c_{00}|00\rangle + c_{10}|10\rangle + c_{01}|01\rangle + c_{11}|11\rangle = \begin{pmatrix} c_{00} \\ c_{01} \\ c_{10} \\ c_{11} \end{pmatrix},$$

$$\text{where } |c_{00}|^2 + |c_{01}|^2 + |c_{10}|^2 + |c_{11}|^2 = 1.$$

$$C = 2|c_{00}c_{11} - c_{10}c_{01}| \quad \text{Entanglement degree} \quad C = 0 \quad \leftrightarrow \quad |\Psi\rangle = |\psi_1\rangle \otimes |\psi_2\rangle.$$



The reversible inverter or *controlled* NOT operator (CNOT) is one of the main two-qubit gates. This gate is described by the 4×4 matrix, which can be represented in the form

$$\text{CNOT} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \otimes \mathbf{1} + \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \otimes \sigma_x = |0\rangle\langle 0| \otimes \mathbf{1} + |1\rangle\langle 1| \otimes \sigma_x,$$

where, $\mathbf{1}$ is the 2×2 identity matrix.

Consider Hamiltonian of the form

$$H = h \otimes 1 + 1 \otimes h + \epsilon A,$$

where $\epsilon \in \{0, 1\}$ and the Hamiltonian h is time independent and has the form

$$h = \begin{pmatrix} a & 0 \\ 0 & b \end{pmatrix}.$$

In this case, if the operator A commutes with $h \otimes 1 + 1 \otimes h$, the evolution operator is represented as

$$\mathcal{U}(t) = (e^{-iht} \otimes e^{-iht})e^{-iAt}.$$

Consider the operator $\exp(-iAt) \equiv R(t)$ in the form

$$R(t) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos(t) & -i\sin(t) & 0 \\ 0 & -i\sin(t) & \cos(t) & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

The matrix $A(t)$ is given by the expression

$$A = i \frac{dR(t)}{dt} R^{-1}(t) = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}.$$

The matrix

$$h = \sigma_3/2 = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

satisfies the commutation condition

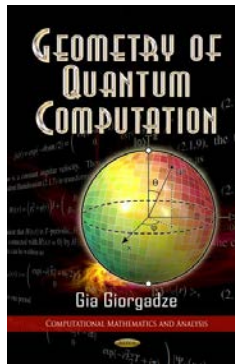
$$[A, (h \otimes 1 + 1 \otimes h)] = 0.$$

Entanglement operator

$$\mathcal{U}(t) = \begin{pmatrix} e^{it} & 0 & 0 & 0 \\ 0 & \cos(t) & -i \sin(t) & 0 \\ 0 & -i \sin(t) & \cos(t) & 0 \\ 0 & 0 & 0 & e^{-it} \end{pmatrix}$$

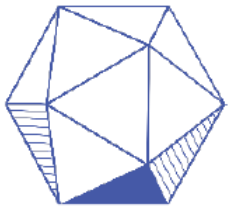
$$\mathcal{U}(t) = (e^{-iht} \otimes e^{-iht}) e^{-iAt}.$$

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THE END

Thanks for Attention !