An approach towards approximation of the Design of Quantum Gate

Shakti Sharma^{1*}, Harish Parthasarathy², Akash Tayal³, Geeta Bhatt¹, Manoj Khanna⁴ and Updesh Sharma⁵

Department of Instrumentation, Bhaskaracharya College of Applied Sciences, Delhi University, New Delhi, India¹ Division of Electronics and Communication, Netaji Subhas Institute of Technology, New Delhi, India² Department of Electronics and Communication Engineering, Indira Gandhi Delhi Technical University for Women,

New Delhi, India³

Department of Electronics, Bhaskaracharya College of Applied Sciences, Delhi University, New Delhi, India⁴ Solid State Physics Lab, Delhi, India⁵

Abstract

Ouantum Gate is a Unitary operator or a Unitary Gate for evolution of a quantum operation which satisfies condition $U^{-1}=U^*$. Quantum gates are different from classical gates. Ouantum gates are always reversible therefore energy loss does not occur between input and output states. Hadamard gate, Phase Gate, CNOT (Controlled NOT) Gate etc are quantum gates. Scattering technique is used to obtain information on the particles therefore applied for evolution. Several algorithms have been developed for quantum computers like Shor's algorithm, Searching algorithms, Fourier transform algorithm. There are various hardware mechanisms are developing through which these gates are tried to be implemented like Ion traps, Quantum Dots, Impurity Atoms, Superconductors etc. In this paper an effort has been done to present a mathematical approach of quantum computer gate design using MATLAB. In this paper, a unitary gate U_d is realized using an atomic system under evolution having Hamiltonian H_0 . After time t, $U_0(t)=exp($ it H_0). H_0 is designed in a way so that $U_0(t) \approx U_d$. Then U_d got perturbed slightly to $U'_d=U_d+\delta U_d$ and extensive efforts have been done to correct the atomic evolution operator $U_0(t)$ so that U'_d is well approximated. For the purpose the atomic evolution theory has been followed by a time independent scattering process with a weak potential εV . Unitarity of evolution is defined by Quantum Fourier Transform algorithm which performs transform of quantum mechanical Fourier amplitudes.

Keywords

Born approximation, Quantum Computation, Quantum Fourier Transform, Quantum Gate, Unitary Gate, Perturbation.

1. Introduction

In quantum theory, information is encoded on spin, polarization etc states of particles like ions, electrons or photons. A physical state is represented by a state vector called 'ket' denoted by $|\alpha\rangle$ in a complex vector space[2,8]. It contains the complete information about the physical state. Bra space is a vector space "dual to" ket space. To every ket $|\alpha\rangle$ there exists a bra, denoted by $\langle \alpha | [2,8]$. A Quantum System is considered as finite dimensional Hilbert space and has a countable orthonormal basis [7].

There is a set of vectors in Hilbert space such that $\langle n' | n \rangle = \delta_{n'n}$ where $|n\rangle = |1\rangle, |2\rangle \dots [1]$. Hamiltonian is the operator corresponding to the total energy of the system which is the sum of the kinetic energy and the potential energy. It is a function of the position and momentum operators. The Position, Momentum, Hamiltonian etc characteristics of a particle are recognized as Observables. These Observables of Hilbert space are Hermitian Operators and can be expressed as $|\psi\rangle = \sum_{n} \psi_{n} |n\rangle$ [1]. The state is described by a state vector ψ , which is a complex linear superposition of all binary states of the bits[12]. Qubit is the quantum mechanical bit. $\{|0\rangle, |1\rangle\}$ is computational basis of Qubit. An arbitrary state in this computational basis is: $|\psi\rangle = \alpha |0\rangle + \beta |1\rangle$, where, α , β are complex numbers, with $|\alpha|^2 + |\beta|^2 = 1$ [6].

^{*}Author for correspondence

Quantum Unitary Gate: Quantum Gate is an Unitary Operator representing a quantum operation or evolution. Unitary linear transformation operator U takes as input state $|\phi\rangle$ and outputs a different state $U^{|\phi\rangle}$. The adjoint of U, denoted U^{\dagger} , is defined by $(U_{\vec{v},\vec{w}}) = (\vec{v}, U^{\dagger}\vec{w})$. In a basis, U^{\dagger} is the conjugate transpose of U. U is unitary if $U^{\dagger} = U^{-1}$ [1,2,4,6,12]. The quantum evolution is always unitary. Incident wave state vector satisfies the time dependent Schrodinger equation [1]

$$i \frac{d}{dt} |\psi_t\rangle = H |\psi_t\rangle$$
 (1)

Hamiltonian H is independent of t, so the general solution of the Schrödinger equation has the form [1,13]

$$|\psi_t\rangle = U(t)|\psi\rangle \equiv e^{-iHt}|\psi\rangle \qquad (2)$$

Here the evolution operator maps the state vector for time zero onto corresponding vector for time t. Since H is self adjoint, the evolution operator U(t) is unitary[1].

2. Modelling of system under study

A particle with mass m and momentum p=ħk, at time t_0 is in the state $|\psi_i\rangle$ is scattered by the potential V to scattered state $|\psi_s\rangle$. Motion of a particle of mass m in a force field V is given by Schrodinger equation[9,10]

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi + V(r,t)\psi$$
⁽³⁾

Since scattering process is Time independent, hence

$$H = H_0 + V \text{ where } \quad H_0 = \frac{p^2}{2m} (4)$$

Incident plane wave can be represented as[11]

$$\left\langle \overrightarrow{r} \mid \psi_{0} \right\rangle = \psi_{0} \left(\overrightarrow{r} \right) = e^{i \overrightarrow{k} \cdot \overrightarrow{r}}$$

$$(5)$$

For localized potential [11] V(r), $r \rightarrow \infty$

The incident state $|\psi_i\rangle$ is an eigenstate of the free particle Hamiltonian H₀ with eigenvalue E. Hence the energy-eigenstate will be [11]

$$\left(E - H_0 - V\right) \left|\psi\right\rangle = 0 \tag{6}$$

Incident particles are weakly interacting with their target, hence multiple scattering is not been considered. Scattering amplitude is calculated using a first order Born approximation[3,9]

$$\psi_{s} = -\frac{1}{4\pi} \frac{2m}{\hbar^{2}} \frac{e^{ikr}}{r} \int d^{3}x' e^{-ik'x'} V(x') \psi_{i} (\mathbf{r}')$$
(7)

The Born Approximation of the scattering amplitude is the Fourier Transform of the scattering potential [3,15]. Final wave is a summation of incident and

scattered wave [3,9]
$$\psi_f = \psi_i + \psi_s$$
(8)

$$\psi_{f} = \psi_{i} - \frac{1}{4\pi} \frac{2m}{\hbar^{2}} \frac{e^{ikr}}{r} \int d^{3}x' e^{-ik'x'} V(x') \psi_{i} (\mathbf{r}')$$
(9)

Fig 1: Incident plane waves, scattered waves and final wave [14]

Potential V is the Yukawa potential which is a Coulomb potential with an exponential drop-off as

$$V(r) = \frac{V_0}{r} \frac{e^{-\mu r}}{\mu}$$
(10)

 $r \rightarrow \infty$ [15]. $r \mu$ (10) Here r is the position vector of a point from potential. The scattering potential is assumed to be generated by a distribution of charge over a small region of space.

$$V(\underline{r}) = \int_{B} \frac{\rho(\underline{r'})}{4\pi\varepsilon_0 |\underline{r} - \underline{r'}|} d^3 r'$$
(11)

For r>>r', above can be approximated by [15]

$$V(r) = \sum_{l=0}^{N} \frac{C_l P_l(\cos \theta)}{r^{l+1}}$$
(12)

Where P_1 are Legendre polynomials. These polynomials can be represented using Rodrigues' formula [5]:

$$P_{l}(x) = \frac{1}{2^{l} l!} \frac{d^{l}}{dx^{l}} (x^{2} - 1)^{l}$$
⁽¹³⁾

These polynomials generate spherical harmonics.



Fig 2: Spherical Harmonics

3. Designing Gate

When the scattering potential is small, the outstate is a small perturbation of the input state.

$$\left| \psi_{f} \right\rangle = \left| \psi_{i} \right\rangle + \varepsilon T_{v} \left| \psi_{i} \right\rangle$$

$$\left| \psi_{f} \right\rangle = \left(I + \varepsilon T_{v} \right) \left| \psi_{i} \right\rangle$$

$$(14)$$

Where Tv is a skew Hermitian operator determined by the potential V. Given a unitary gate U_d which is like the Fourier Transform

$$\tilde{\tilde{U}}_{d} = \frac{1}{\sqrt{N}} \left\| \exp\left(\frac{j2\pi kn}{N}\right) \right\|_{0 \le k, n \le N-1}$$
(15)

We design V so that

$$I + \varepsilon T_{v} = U_{d}^{1/k}$$
(16)

Where k is a large integer. V is selected so that $||I+\epsilon Tv-Ud||$ is a minimum. V is taken as a multipole potential of the form

$$V(r,\theta) = \sum_{l=0}^{N} \frac{c(l)P_{l}(\cos\theta)}{r^{l+1}}$$
(17)

Then Tv is of the form

$$Tv = \sum_{l=0}^{N} c(l) V_l(r, \theta) \equiv \sum_{l=0}^{N} c(l) V_l(r)$$
(18)

Where $V_l(r,\theta)$ is completely determined by the

$$\hbar ki = \hbar k ni$$

projectile moment – . The finite dimensional approximation is chosen by taking the

initial state
$$\psi_i(\underline{r}) = C \cdot \exp\left(jk \hat{n_i} \cdot \underline{r}\right)$$

Using Born scattering, the final state is given by

$$\psi_i^f\left(\frac{r}{r}\right) = \frac{\delta \cdot m_0 C}{2\pi\hbar^2} \int V\left(\frac{r}{r}\right) \psi_i\left(\frac{r}{r}\right) \frac{\exp\left(jk\left|\frac{r}{r}-\frac{r}{r}\right|\right)}{\left|\frac{r}{r}-\frac{r}{r}\right|} d^3r' + \psi_i\left(\frac{r}{r}\right)$$

$$\psi_{f}\left(\underline{r}\right) = \int k\left(\underline{r}, \underline{r}\right) \psi_{i}\left(\underline{r}\right) d^{3}r^{2}$$

the kernel of this transformation is

$$k\left(\underline{r},\underline{r}'\right) = \delta\left(\underline{r},\underline{r}'\right) + \frac{\delta \cdot m_0}{2\pi\hbar^2} \frac{\exp\left(jk\left|\underline{r}-\underline{r}'\right|\right)}{\left|\underline{r}-\underline{r}'\right|} V\left(r'\right)$$

$$k=I+\delta\sum_{l=0}^{N}C(l)T_{l}$$

We choose
$$\{C(l)\}$$
 so that

$$E\left(\left\{\mathbf{C}(1)\right\}_{0}^{N}\right) = \left\|I - U_{d} + \delta \sum_{l=0}^{N} C(l)T_{l}\right\|^{2}$$

is a minimum.

(19)

$$E(\{C(l)\}) = \left\|I - U_d\right\|^2 + \delta^2 \sum_{l,m=0}^N C(l)C(m)Ir(I_l^*T_m) - 2\delta \sum_{l=0}^N C(l)\operatorname{Re}Ir((I - \operatorname{Ud})I_l^*)$$

$$\frac{\partial E}{\partial C(l)} = \mathbf{O}$$

$$\delta \sum_{m=0}^{N} Tr(T_l * T_m) C(m) = \operatorname{Re}(Tr((I - U_d)T_l *))$$

$$R = ((Tr(T_l^* T_m)))_{0 \le l, m \le N}$$

and
$$E = ((\operatorname{Re}Tr((I - U_d)T_l^*)))_{0 \le l \le N}$$

Gives

$$RC = \delta^{-1} E$$
or
$$C = \delta^{-1} R^{-1} E$$
(20)

C(l)'s are chosen so that the average error energy between the desired set of final states and the actual set of final states is a minimum.

Scattering process parameters are listed in table 1.

Table 1: Scattering process parameters

| Parameters | Value |
|---|---------------|
| ' λ ' Wavelength of incident wave | 1 Armstrong |
| 'm' Mass of particle | 9.1*10^-31 kg |
| 'r' position vector of source | 15 micron |
| 'r' position vector of Detector | 1 micron |

4. Result

Incident wave, Scattered wave and Final wave patterns in fig 3 are plotted using MATLAB code. The perturbed wave after scattering showing decay in amplitude for various ' θ ' and ' ϕ ' values.



Fig 3: Incident coordinates θ =90°, ϕ =180°, iteration=20.

These wave patterns are obtained for various number of incident particles for fixed 'r' but different θ and φ . Since source is considered at larger distance, therefore the incident waves are forming plane waves. This is a time independent scattering process which is required for the atomic evolution. Scattered waves can be represented as a hankle function which is a multipole expansion. The harmonics are visible at corners and are spherical in nature. Scattering amplitude is obtained using First order Born approximation which is a Fourier Transform representation and its kernel is of unit magnitude. The superposition of incident and scattered wave is forming a final wave pattern in such a manner that is similar to the incident plane wave.

5. Conclusion and Future Work

Decoherence, Noise and Hardware Design are main limitations of a quantum computational system. Quantum state of a particle can be easily changed due to interaction with its environment. In our study, only momentum of particle is taken into consideration. Scattering potential is static potential and chosen very weak and multiple scattering is not considered. First order born approximation is taken for calculation to approximate amplitude of scattered wave. Enormous scope of study is present in this field in future. Multiple scattering and different potentials can be taken further and more precise Gates can be designed for realistic targets.

References

- [1] Taylor, John R. Scattering theory: the quantum theory of nonrelativistic collisions. Courier Corporation, 2012.
- [2] Sakurai, J. J., and J. J. Napolitano. knjige ili časopisa:* Modern Quantum Mechanics. 1985.
- [3] Harish Parthasarathy, "Applications of Advanced Signal Analysis", I.K International Publishing House, 2011.
- [4] Kato, Tosio. Perturbation theory for linear operators. Springer Science & Business Media, 2012.
- [5] Jackson, John David, and John D. Jackson. Classical electrodynamics. Vol. 3. New York etc.: Wiley, 1962.
- [6] Nielsen, Michael A., and Isaac L. Chuang. Quantum computation and quantum information. Cambridge university press, 2010.
- [7] Prugovečki, Eduard. Quantum mechanics in Hilbert space. Vol. 41. Academic Press, 1971.

- [8] Dirac, Paul Adrien Maurice. The principles of quantum mechanics. No. 27. Oxford university press, 1981.
- [9] Feynman, Richard Phillips, and Albert R. Hibbs. Quantum mechanics and path integrals. Vol. 2. New York: McGraw-Hill, 1965.
- [10] Feynman, Richard Phillips, and Albert R. Hibbs. Quantum mechanics and path integrals. Vol. 2. New York: McGraw-Hill, 1965.
- [11] Kuroda, Shige Toshi. An introduction to scattering theory. No. 51. Matematisk Institut, Aarhus Universitet, 1978.
- [12] Barenco, Adriano, et al. "Elementary gates for quantum computation." Physical Review A 52.5 (1995): 3457.
- [13] Altafini, Claudio. "On the generation of sequential unitary gates from continuous time Schrödinger equations driven by external fields." Quantum Information Processing 1.3 (2002): 207-224.

- [14] Taylor, John R. "Scattering theory." (1972).
- [15] Alexander Altland, "Advanced Quantum Mechanics", 2013.



Shakti Sharma is an Assistant Professor in the Department of Instrumentation, Bhaskaracharya College of Applied Sciences, Delhi University, New Delhi, India. She did her M.Sc. in Electronics from Devi Ahilya University, Indore and M.Tech. in Electronics and Communication

Engineering from Guru Gobind Singh Indraprastha University, Delhi. Her area of interest are Digital Signal Processing, MEMS Technolgy and Quantum Computing. Email: shaktisharma2007@gmail.com