Abstract

Genetic algorithms (GA) are stochastic global search methods based on the mechanics of natural biological evolution, proposed by John Holland in 1975. Here in this thesis, we have exploited possible utilities of Genetic Algorithm optimization in Nuclear Magnetic Resonance (NMR) experiments. We have performed (i) Pulse sequence generation and optimization for NMR Quantum Information Processing, (ii) efficient creation of NOON states, (iii) Composite operator design and (iv) delay optimization for refocused quantitative INEPT. We have generated time optimal as well as robust pulse sequences for popular quantum gates. A Matlab package is developed for basic Target unitary operator to pulse sequence optimization and is explained with an example.

Chapter 1 contains a brief introduction to NMR, Quantum computation and Genetic algorithm optimization. Experimental unitary operator decomposition using Genetic Algorithm is explained in Chapter 2. Starting from a two spin homonuclear system (5-Bromofuroic acid), we have generated hard pulse sequences for performing (i) single qubit rotation, (ii) controlled NOT gates and (iii) pseudo pure state creation, which demonstrates universal quantum computation in such systems. The total length of the pulse sequence for the single qubit rotation of an angle $\pi/2$ is less than 500$\mu$s, whereas the conventional method (using a selective soft pulse) would need a 2$ms$ shaped pulse. This substantial shortening in time can lead to a significant advantage in quantum circuits. We also demonstrate the creation of Long Lived Singlet State and other Bell states, directly from thermal equilibrium state, with the shortest known pulse sequence. All the pulse sequences generated here are generic i.e., independent of the system and the spectrometer.

We further generalized this unitary operator decomposition technique for a variable operators termed as Fidelity Profile Optimization (FPO) (Chapter 3) and performed quantum simulations of Hamiltonian such as Heisenberg XY interaction and Dzyaloshinskii-Moriya interaction. Exact phase ($\phi$) dependent experimental unitary decompositions of Controlled-$\phi$ and Controlled Controlled-$\phi$ are solved using first order FPO. Unitary operator decomposition for experimental quantum simulation of Dzyaloshinskii-Moriya interaction in the presence of Heisenberg XY interaction is solved using second order FPO for any relative strengths of interactions ($\gamma$) and evolution time ($\tau$). Experimental gate time for this decomposition
is invariant under $\gamma$ or $\tau$, which can be used for relaxation independent studies of the system dynamics. Using these decompositions, we have experimentally verified the entanglement preservation mechanism suggested by Hou et al. [Annals of Physics, 327 292 (2012)].

NOON state or Schrodinger cat state is a maximally entangled $N$ qubit state with superposition of all individual qubits being at $|0\rangle$ and being at $|1\rangle$. NOON states have received much attention recently for their high precession phase measurements, which enables the design of high sensitivity sensors in optical interferometry and NMR [Jones et al. Science, 324 1166(2009)]. We have used Genetic algorithm optimization for efficient creation of NOON states in NMR (Chapter 4). The decompositions are, $(i)$ a minimal in terms of required experimental resources – radio frequency pulses and delays – and have $(ii)$ good experimental fidelity.

A composite pulse is a cluster of nearly connected $rf$ pulses which emulate the effect of a simple spin operator with robust response over common experimental imperfections. Composite pulses are mainly used for improving broadband decoupling, population inversion, coherence transfer and in nuclear overhauser effect experiments. Composite operator is a generalized idea where a basic operator (such as rotation or evolution of $zz$ coupling) is made robust against common experimental errors (such as inhomogeneity / miscalibration of $rf$ power or error in evaluation of $zz$ coupling strength) by using a sequence of basic operators available for the system. Using Genetic Algorithm optimization, we have designed and experimentally verified following composite operators, $(i)$ broadband rotation pulses, $(ii)$ $rf$ inhomogeneity compensated rotation pulses and $(iii)$ $zz$ evolution operator with robust response over a range of $zz$ coupling strengths (Chapter 5). We also performed $rf$ inhomogeneity compensated Controlled NOT gate.

Extending Genetic Algorithm optimization in classical NMR applications, we have improved the quantitative refocused constant-time INEPT experiment (Q-INEPT-CT) of Mäkelä et al. [JMR 204(2010) 124-130] with various optimization constraints. The improved ‘average polarization transfer’ and ‘min-max difference’ of new delay sets effectively reduces the experimental time by a factor of two (compared with Q-INEPT-CT, Mäkelä et al.) without compromising on accuracy (Chapter 6). We also introduced a quantitative spectral editing technique based on average polarization transfer. These optimized quantitative experiments are also described in Chapter 6.
Time optimal pulse sequences for popular quantum gates such as, (i) Controlled Hadamard (C-H) gate, (ii) Controlled-Controlled-NOT (CCNOT) Gate and (iii) Controlled SWAP (C-S) gate are optimized using Genetic Algorithm (Appendix. A). We also generated optimal sequences for Quantum Counter circuits, Quantum Probability Splitter circuits and efficient creation of three spin W state. We have developed a Matlab package based on GA optimization for three spin target operator to pulse sequence generator. The package is named as UOD (Unitary Operator Decomposition) is explained with an example of Controlled SWAP gate in Appendix. B.

An algorithm based on quantum phase estimation, which discriminates quantum states non-destructively within a set of arbitrary orthogonal states, is described and experimentally verified by a NMR quantum information processor (Appendix. C). The procedure is scalable and can be applied to any set of orthogonal states. Scalability is demonstrated through Matlab simulation.