A quantum control algorithm: Models and theory

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Abstract

The Schrödinger equation: $\left(-\frac{\hbar^2}{2m}\nabla^2 + \hat{V}(x)\right)\Psi(x,t) = i\hbar\partial_t\Psi(x,t)$. In NMR spectroscopy, the kinetic term $-\frac{\hbar^2}{2m}\nabla^2$ can be abbandoned an $\hat{V}(x)$ splits in H_d and H_c, where H_d can be diagonalised and H_c has a recursive shape. In order to overlap the time propagation $U(t) = e^{-i\hat{H}\Delta t}$ with the desired matrix U_G, a gradient flow algorithm can be utilized. This leads to some numerical challenges thus as calculating a matrix exponential as well as producing the product of many matrices.
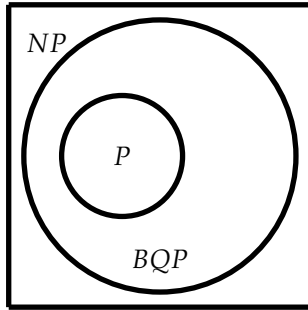
Figure 1: Illustration of prominent problem classes

1 Introduction

1.1 Quantum computing

A quantum computer uses so called qubits instead of traditional bits to solve some problems more efficiently than on classical hardware:

- Integer factorization is one way to break the popular crypographic algorithm RSA. The best known algorithm on traditional hardware runs in $\mathcal{O}\left(\exp\left(\left(\frac{64}{9}b\right)^{\frac{1}{3}}(\log b)^{\frac{2}{3}}\right)\right)$ (General number field sieve (GNFS)). Shor's prime factorisation would run in polynomial time, if a quantum computer would be available to run it.

- Traditional array searches run in $\mathcal{O}(n)$, whereas the Grover-Algorithm gets the job done in $\mathcal{O}(\sqrt{n})$.

- Quantum-Simulation: to simulate quantum systems, it is obviously a good choice to use quantum systems.

Quantum control plays a key role in quantum technology, as quantum gates aren't hardwired as in traditional chips, but sophisticated manipulations of quantum systems. These quantum gates have to be calculated very precisley as it is their purpose to bring the system in a defined state

1.2 What is not possible

The class of problems a quantum computer can solve in polynomial time with an error propability of less than $1/4$ is called BQP. It is known, that $P \subseteq BQP$ and that BQP is a subset of NP. However, it is not known, if BQP is a true subset of NP, which would yield that $P \neq NP$ and therefore solve the $P = NP$ problem. Another problem is the feasibility: The biggest approved quantum register realized up to now could hold 8 qubits and therefore quantum computing is no realistic option for real problems in the next couple of years. For instance, to factorize a n bit integer, you need up to $2 \cdot \lceil \log_2(n) \rceil$ qubits.

2 Physics

2.1 Classic mechanics

Newton law states $F = m \cdot \ddot{x}$, where m is the mass, $\ddot{x}$ the acceleration and F the resulting force.[1] Disregarding friction, this can be shown to be equivalent to $\frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{x}} - \frac{\partial \mathcal{L}}{\partial x} = 0$ with $\mathcal{L} = \frac{1}{2} \cdot m \cdot \dot{x}^2 - V(x)$ ($V(x)$ is the potential energy) being the Lagrange-Function. Hamilton has shown that the Lagrange equation is equivalent to this system of two partial differential equations:

- $\dot{p} = -\frac{\partial H}{\partial x}$
- $\dot{x} = \frac{\partial H}{\partial p}$

With p being the momentum $p = m \cdot \dot{x} = \frac{\partial \mathcal{L}}{\partial \dot{x}}$ and $H = \frac{1}{2}m\dot{x}^2 + V(x) = \frac{p^2}{2m} + V(x)$ being the energy of the system.

2.2 Quantum Mechanics

In classical physics, $x(t)$ is a function which describes the trajectory of a mass point exactly. In quantum mechanics $x(t)$ is replaced by the wave function $\Psi(x, t)$. *The Correspondence principle* Classical functions become operators on the wave function whose eigenvalues are the observable values. In position space, this yields $x \rightarrow \hat{x}$, $p \rightarrow -i\hbar\nabla$ and $E \rightarrow i\hbar\partial_t$. This substitution is due to the correspondence principle, which is not really the source but a consequence of quantum mechanics.[2] Applied to the Hamilton equation this yields the Schrödinger equation $(-\frac{\hbar^2}{2m}\nabla^2 + \hat{V}(x))\Psi(x, t) = i\hbar\partial_t\Psi(x, t)$.

2.3 Spin

2.3.1 Discovery

In 1922, Otto Stern and Walther Gerlach made an experiment with accelerated silver-atoms in an inhomogenous magnetic field and found that the ray got split in two parts along the magnetic field axis. This was unexpected since the only relevant $5s$ valence electron has no orbital angular momentum and hence no magnetic dipole moment which could interact with the magnetic field. Today we know that electrons have an intrinsic attribute we call spin and which is correlated with a magnetic dipole moment with the so called g-factor. Spin is not simple angular momentum, because electrons are point-shaped and have no volume (as far as we know). The schrödinger equation does not predict spin as there is no classical analogon to it and we derived the equation by applying the correspondence principle to the Hamilton function. To completly understand spin, one has to do relativistic calculations and use the Dirac equation, but this is beyond the scope of this paper.

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[1] As we know today, this is just an approximation. In cases, where high velocities are involved, one should use Einstein's theory of special relativity.

[2] But this way, it is simpler to understand

2.3.2 The Spin operator

Let z be the distinguished axis. From the Stern-Gerlach experiment we know that the eigenvalues of $\hat{S}_z$ have to be $\pm\frac{\hbar}{2}$. Hence there have to be two different linear independent eigenvectors which we call (for historical reasons) $|\uparrow\rangle$ and $|\downarrow\rangle$. Therefore we can write the spin state of our electron as a complex linear combination of these two vectors.

$$\begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \alpha |\uparrow\rangle + \beta |\downarrow\rangle \in \mathbf{C}^2$$

Because $|\alpha|^2$ equals the propability of finding $|\uparrow\rangle$ in an experiment and $|\beta|^2$ equals the propability of finding $|\downarrow\rangle$, the normation condition is $|\alpha|^2 + |\beta|^2 = 1$.

2.3.3 The Pauli spin matrices

In analogy to classic angular momentum, the spin operator has to satisfy $[\hat{S}_x, \hat{S}_y] = i\hbar\hat{S}_z$ and cyclical with $[A, B] := AB - BA$ being the commutator. The spin operators in the three dimensions can be written as matrices:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

With $\hat{S}_i = \frac{\hbar}{2}\sigma_i$.

2.4 Coupled Spins

In order to couple two spins in one system, one has to calculate the kronecker product of these two systems. Therefore we yield $2^2 = 4$ new basis vectors:

$$|\uparrow\rangle \otimes |\uparrow\rangle =: |\uparrow\uparrow\rangle \tag{1}$$
$$|\uparrow\rangle \otimes |\downarrow\rangle =: |\uparrow\downarrow\rangle \tag{2}$$
$$|\downarrow\rangle \otimes |\uparrow\rangle =: |\downarrow\uparrow\rangle \tag{3}$$
$$|\downarrow\rangle \otimes |\downarrow\rangle =: |\downarrow\downarrow\rangle \tag{4}$$

In general, one can couple n spins by producing the kronecker product of all basis vectors, yielding 2^n basic states. The potential between two spins is direct proportional to the scalar product of the two spin operators or to be more exactly their eigenvalues:

$$\hat{V} = \mu\hat{S}^{(1)} \circ \hat{S}^{(2)} = \mu\left(\hat{S}_z^{(1)} \otimes \hat{S}_z^{(2)} + \frac{1}{2}\left(\hat{S}_+^{(1)} \otimes \hat{S}_-^{(2)} + \hat{S}_-^{(1)} \otimes \hat{S}_+^{(2)}\right)\right)$$

With μ being a constant and $\hat{S}_\pm = \hat{S}_x \pm i\hat{S}_y$ with the attributes

$$\hat{S}_+ |\uparrow\rangle = 0 \qquad \hat{S}_+ |\downarrow\rangle = \hbar |\uparrow\rangle \tag{5}$$
$$\hat{S}_- |\uparrow\rangle = \hbar |\downarrow\rangle \qquad \hat{S}_- |\downarrow\rangle = 0 \tag{6}$$

We can describe the complete potential of a system by a hermitian $2^n \times 2^n$ matrix with vanishing trace.

Figure 2: 900MHz, 21.2 T NMR Magnet at HWB-NMR, Birmingham, UK; credit: wikipedia

3 Nuclear magnetic resonance

3.1 preposition

Nuclei of atoms have like electrons their own spin. One can couple multiple spins in an experimental setup and manipulate them by external magnetic fields. Spins can be measured by stimulated emission of radiaton The technical challenges include the creation of very strong magnetic fields ($\approx$ 20T) and the compensation of the energy relaxation as well as avoiding of the decoherence. Each physical system propagates towards it's energetic ground state. This energy relaxation called phenomen erases the qubits after a certain amount of time, which makes the quantum computer unusable. Also, the superposition of multiple spins can be destroyed by interaction with the environment; this is called decoherence and to avoid it, one has to isolate the experimental setup very carefully from the outside.

3.2 Some Physics

We remember the Schrödinger equation:

$$\hat{H}\Psi(x,t) = \left(-\frac{\hbar^2}{2m}\nabla^2 + \hat{V}(x)\right)\Psi(x,t) = i\hbar\partial_t\Psi(x,t)$$

In our case, the particles don't move, so we can abbandon the kinetic term $-\frac{\hbar^2}{2m}\nabla^2$. We already know the potential for two particles. For n particles, this yields

$$\hat{V}(x) = \frac{1}{2}\sum_{i\neq j}\mu_{ij}\hat{S}^{(i)}\circ\hat{S}^{(j)}$$

This is a $2^n \times 2^n$ matrix which can be diagonalised. In the following, we will refer to this diagoalised matrix as H_d. Previously we stated that the spin system can be controlled by external magnetic fields. In our formal model this can be read as application of the $\hat{S}_{\pm}$ operators on single spins. For n spins which can be separatley influenced, the controlled potential is

$$\hat{V}_c = \sum_{k=0}^{n-1}\left(u_k(\cdot\mathbb{1}_{2^k}\otimes\sigma_x\otimes\mathbb{1}_{2^{n-k-q}} + i\cdot\mathbb{1}_{2^k}\otimes\sigma_y\otimes\mathbb{1}_{2^{n-k-q}})\right)$$
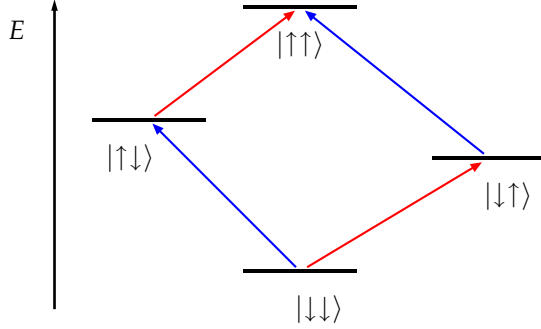
Figure 3: Induced spinflips in a two particle system: red is $\mathbb{1}_2 \otimes \hat{S}_+$ and blue is $\hat{S}_+ \otimes \mathbb{1}_2$.

Which we will call H_c. One can build the matrix of H_c for n particles using the following recursion:

$$A_{n+1} = \left(\begin{array}{cc} A_n & \mathbb{1}_{2^n} \\ \mathbb{1}_{2^n} & A_n \end{array} \right)$$

With $A_0 = (0)$ being the matrix for zero particles.

3.3 The GRAPE algorithm

3.3.1 The solution of the Schrödinger equation

The time-independent Schrödinger equation $i\hbar\partial_t\Psi = \hat{H}\Psi$ (in the Gaussian system: $i\partial_t\Psi = \hat{H}\Psi$) has the solution: $\Psi(t) = e^{-i\hat{H}t}\Psi(0)$. With the matrix exponential function $e^{\hat{H}} = \sum_{k=0}^{\infty} \frac{\hat{H}^k}{k!}$. Our Hamiltonian was: $\hat{H} = H_d + H_c(u_1(t),\ldots) = H_d + \sum_j H_j(t)$ With $H_j(t)$ piecewise constant on $t + \Delta t$. So in our case the solution is: $\Psi(t) = e^{-i\Delta t \hat{H}(t_k)}e^{-i\Delta t \hat{H}(t_{k-1})}\cdots e^{-i\Delta t \hat{H}(t_1)}\Psi(0) =: U(t)\Psi(0)$ With $k\Delta t = t$.

3.3.2 Quantum gate construction

A quantum gate is an operation on the spin state of the system which performs a desired change in it, e.g. NOT, NAND, XOR,.... For each of these gates the desired operation can be described by a matrix U_G. So the challenge is: adjusting $H_j(t_k)$ so that $U(t)$ overlaps best with U_G for a given time $t = T$. It can be shown that maximising $\Re\ tr(U_G^\dagger U(T))$ subject to $\partial_t U(t) = -i\hat{H}U(t)$ optimizes the propagator. To solve this task, Khajena and Glaser came up with a gradient flow algorithm they called "gradient ascent pulse engineering" (GRAPE):
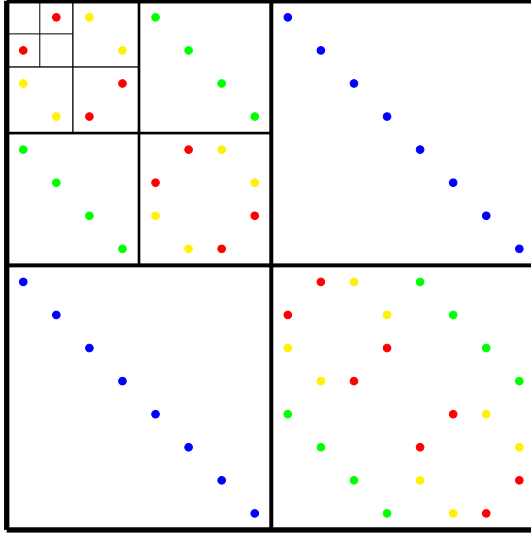
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Figure 4: The control term for a 4 spin system: Each dot stands for a non-zero entry in the matrix; The recursion can be seen, starting from the top left corner where $A_0 = 0$ resides. The next bigger rectangle has this in its main diagonal and the identity in its secondary diagonal. And so on.

1. Set initial controls $u_j^{(r)}(t_k)$ for all times t_k ($k \in \{1, 2, \ldots, M\}$) at random or by guess

2. **For each** $k \in \{1, \ldots, M\}$ **do**:
   (a) Calculate the forward-propagation $U(t_k) = e^{-i\Delta t \hat{H}(t_k)} e^{-i\Delta t \hat{H}(t_{k-1})} \ldots e^{-i\Delta t \hat{H}(t_1)}$
   (b) Calculate the backward-propagation $\Lambda(t_k) = e^{-i\Delta t \hat{H}(t_k)} e^{-i\Delta t \hat{H}(t_{k+1})} \ldots e^{-i\Delta t \hat{H}(t_M)}$
   (c) Update $u_j^{(r+1)}(t_k) = u_j^{(r)}(t_k) + \varepsilon \Re \left(tr \left(\Lambda^\dagger(t_k)(-i\hat{H}_j)U(t_k) \right) \right)$

3. Return to step 2 with the new controls $u_j^{(r+1)}$

One can set the initial controls found with other algorithms, e.g. CORPSE or short-CORPSE (SCORPSE), but this is not really necessary since GRAPE will always find the nearest local optimum to its starting position. But Note: It can never be proven that the global optimum is found, so we shall reference the resulting controls as optimized rather than optimal.

3.3.3 Challenges of GRAPE

GRAPE converges to a local optimum of $U(t)$. It is necessary to re-run it a couple of times with different initial values to confirm that the global maximum is reached altough this cannot be proven. GRAPE also brings some computational challenges, as it requires it's user to calculate the exponential of multiple sparse matrices $U_k := e^{-i\Delta t \hat{H}(t_k)}$ as well as the product of many different matrices $U(t_k) = U_k \cdot U_{k-1} \cdots U_1$ in each step.

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