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A quantum control algorithm: Models and theory

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Outline

Introduction

Physics

Nuclear magnetic resonance

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Quantum computing

Computing

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Control

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.

What is not possible

Complexity

- BQP: The class of problems a quantum computer can solve in polynomial time with an error propability of less than $1/4$.

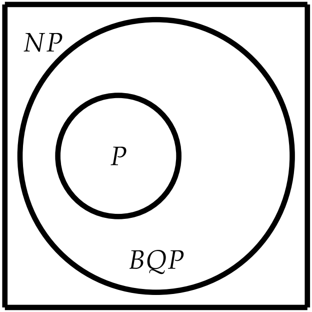

Figure: Illustration of prominent problem classes

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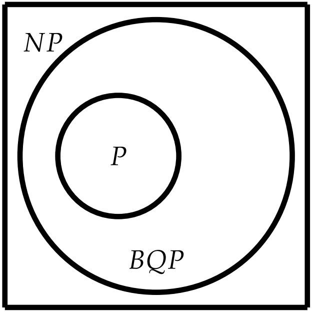

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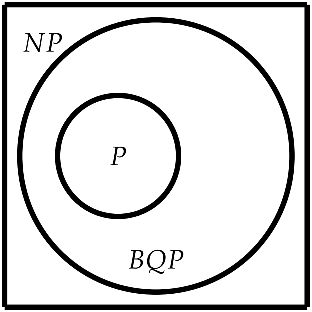

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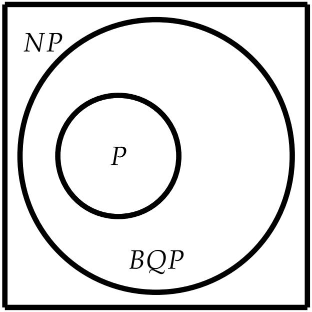
- It is known, that $P \subseteq BQP$.
- Though BQP is a subset of NP, it is not known if it is a true subset.
- Proof that $BQP \subsetneq NP$ would yield that $P \neq NP$ and therefore solve the $P = NP$ problem.



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- Classic mechanics
- Quantum Mechanics
- Spin
- Coupled Spins

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Newton and Lagrange

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Hamilton

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

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The wave function

- In classical physics, $x(t)$ is a function which describes the trajectory of a mass point exactly.
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Classical functions become operators on the wave function whose eigenvalues are the observable values. In position space, this yields $x \longrightarrow \hat{x}$, $p \longrightarrow -i\hbar\nabla$ and $E \longrightarrow i\hbar\partial_t$.

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The Schrödinger equation

Applied to the Hamilton equation this yields the Schrödinger equation
$(-\frac{\hbar^2}{2m}\nabla^2 + \hat{V}(x))\Psi(x,t) = i\hbar\partial_t\Psi(x,t)$

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- Spin is ***not*** angular momentum
- The Schrödinger equation does not directly inhibit spin. To save us from relativistics, we apply it as a hack

The Spin Operator

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

- 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 $|\alpha|^2 + |\beta|^2 = 1$.

The Pauli spin matrices

From vector to matrix

- 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.

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- The spin operators in the three dimensions can be written as matrices:

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

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- We can test our commutator relation from above:

$$[\hat{S}_x, \hat{S}_y] = \frac{\hbar^2}{4}\left(\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} - \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\right)$$

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Coupled systems

The Kronecker tensorproduct

- 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:

$$|\uparrow\rangle \otimes |\uparrow\rangle =: |\uparrow\uparrow\rangle \tag{1}$$

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

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- In general, one can couple n spins by producing the kronecker product of all basis vectors, yielding 2^n basic states.

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

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

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

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Nuclear magnetic resonance

NMR

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- Decoherence: The superposition of the spins is destroyed by interaction with the environment ("‘super selection rule"’)

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NMR and the Schrödinger equation

We remember

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

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- This is a $2^n \times 2^n$ matrix which can be diagonalised. In the following, we will refer to this diagnoalised matrix as H_d

The control term (1)

How to control our system

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.

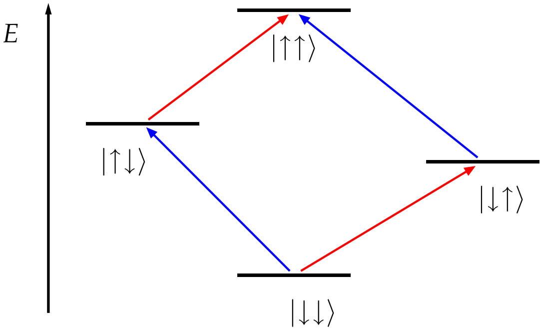

Figure: Induced spinflips in a two particle system: red is $\mathbb{1}_2 \otimes \hat{S}_+$ and blue is $\hat{S}_+ \otimes \mathbb{1}_2$.

The control term (2)

In general

For n spins which can be separatley influenced, the controlled potential is

$$\hat{V}_c = \sum_{k=0}^{n-1} (a_k \cdot \mathbb{1}_{2^k} \otimes \sigma_x \otimes \mathbb{1}_{2^{n-k-q}} + b_k \cdot \mathbb{1}_{2^k} \otimes \sigma_y \otimes \mathbb{1}_{2^{n-k-q}})$$

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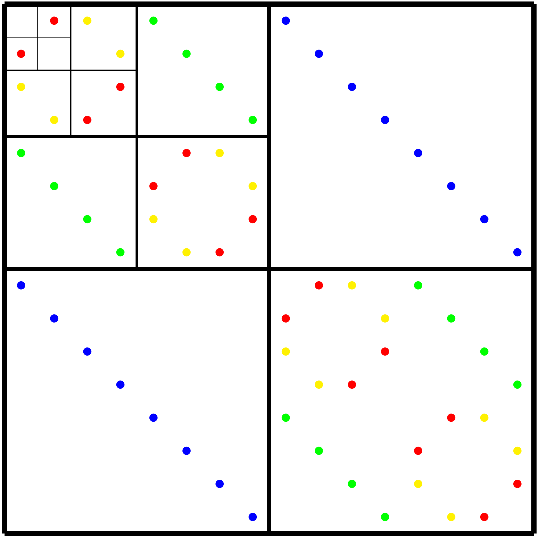
Recursion

One can build the matrix of H_c for n particles using the following recursion:

$$A_{n+1} = \begin{pmatrix} A_n & \mathbb{1}_{2^n} \\ \mathbb{1}_{2^n} & A_n \end{pmatrix}$$

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

Eye candy



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- Our Hamiltonian was: $\hat{H} = H_d + H_c(a_1(t), b_1(t), \ldots) = H_d + H_c(u_1(t), \ldots) = H_d + \sum_j H_j(t)$ With $H_j(t)$ piecewise constant on $t + \Delta t$

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- So in our case the solution is: $\Psi(t) = e^{-i\Delta t\hat{H}(t_k)}e^{-i\Delta t\hat{H}(t_{k-1})} \ldots e^{-i\Delta t\hat{H}(t_1)}\Psi(0) =: U(t)\Psi(0)$ With $k\Delta t = t$

Quantum gate construction

Problem description

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The GRAPE algorithm

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.

GRAPE

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**:
   2.1 Calculate the forward-propagation $U(t_k) = e^{-i\Delta t \hat{H}(t_k)} e^{-i\Delta t \hat{H}(t_{k-1})} \ldots e^{-i\Delta t \hat{H}(t_1)}$
   2.2 Calculate the backward-propagation $\Lambda(t_k) = e^{-i\Delta t \hat{H}(t_k)} e^{-i\Delta t \hat{H}(t_{k+1})} \ldots e^{-i\Delta t \hat{H}(t_M)}$
   2.3 Update $u_j^{(r+1)}(t_k) = u_j^{(r)}(t_k) + \varepsilon \Re \left(tr \left(\Lambda^\dagger(t_k)(-i\hat{H}_j)U(t_k)\right)\right)$
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- One has to calculate the product of many different matrices $U(t_k) = U_k \cdot U_{k-1} \cdots U_1$
- One has to calculate the trace $tr\{(U_k U_{k+1} \cdots U_M)(-i\hat{H}_j)(U_k U_{k-1} \cdots U_1)\} \forall j, k$

Conclusion

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- This leads to some numerical challenges thus as calculating a matrix exponential as well as producing the product of many matrices

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$\forall x,y,z \in V, \forall \lambda \in F$
Then V is a Lie algebra.

Lie algebra (2)

Examples

- The well-known $\mathbb{R}^3$ with the cross product.
- Our previously defined Pauli-Matrices.

Kronecker product (1)

Definition

Let $A \in \mathcal{C}^{m \times n}$, $B \in \mathcal{C}^{r \times s}$. Then the Kronecker product $A \otimes B \in \mathcal{C}^{mr \times ns}$ of A and B is defined as:

$$A \otimes B = \begin{pmatrix} a_{11} & \cdots & a_{1n} \\ \vdots & \ddots & \vdots \\ a_{m1} & \cdots & a_{mn} \end{pmatrix} \otimes B := \begin{pmatrix} a_{11}B & \cdots & a_{1n}B \\ \vdots & \ddots & \vdots \\ a_{m1}B & \cdots & a_{mn}B \end{pmatrix}$$

Attributes (1)

- Bilinearity:
  - $A \otimes (B + C) = A \otimes B + A \otimes C$
  - $(A + B) \otimes C = A \otimes C + B \otimes C$
  - $\lambda(A \otimes B) = (\lambda A) \otimes B = A \otimes (\lambda B)$
- associativity: $A \otimes (B \otimes C) = (A \otimes B) \otimes C$

Kronecker product (2)

Attributes (2)

- transposition: $(A \otimes B)^T = A^T \otimes B^T$
- $\forall A, B \in \mathbb{C}^{n \times n},\ C, D \in \mathbb{C}^{m \times m}: \quad (AB) \otimes (CD) = (A \otimes C)(B \otimes D)$
- The kronecker product of diagonal matrices is a diagonal matrix
- $\mathbb{1}_{2^q} = \underbrace{\mathbb{1}_2 \otimes \cdots \otimes \mathbb{1}_2}_{\text{q times}}$
- $tr(A \otimes B) = tr(A) \cdot tr(B)$

Drift-Term

Two spin system

$$|\Psi_1\rangle := |\uparrow\uparrow\rangle \quad |\Psi_2\rangle := |\uparrow\downarrow\rangle \quad |\Psi_3\rangle := |\downarrow\uparrow\rangle \quad |\Psi_4\rangle := |\downarrow\downarrow\rangle$$

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

Non-diagonalised Hamiltonian for two-spin system

$$\hat{H}_d = \frac{\hbar^2}{4}\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 2 & 0 \\ 0 & 2 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

Reference: Myself, so it could be faulty.

Shor's Algorithm (1)

Factorize a number n

1. Pick random $1 < x < n$
2. If $gcd(x, n) > 1 \rightarrow$ **success**
3. Use the period-finding subroutine to find r, the period of $f(v) = x^v \mod n$ i.e. the smallest integer r for which $f(v + r) = f(v)$ (quantum stuff here)
4. If r is odd $\rightarrow$ go back to step 1
5. If $x^{\frac{r}{2}} = -1 \mod n \rightarrow$ go back to step 1
6. $gcd(x^k - 1, n)$ is a nontrivial factor of n. **success**

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Period finding subroutine

You will need at least Q qubits, where $n^2 \leq Q < 2n^2$.

1. Initialize the qubits to $Q^{-\frac{1}{2}} \sum_{x=0}^{Q-1} |x\rangle |0\rangle$
2. Construct $f(x)$ as a quantum function and apply it to the state, to obtain
$$Q^{-\frac{1}{2}} \sum_{x} |x\rangle |f(x)\rangle$$
3. Apply the quantum Fourier transform to get the final state
$$Q^{-1} \sum_{x} \sum_{y} \omega^{xy} |y\rangle |f(x)\rangle$$
4. Perform a measurement. We obtain an equally distributed multiple of $f(x)/r$.
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Stern Gerlach experiment