Linear Algebra Operations in a Quantum Control Problem

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Outline

1) Classical mechanics
2) Quantum Mechanics
3) Schrödinger equation
4) Spin and its Equations
5) Spin coupling
6) NMR
7) Matrix exponential
8) Algorithms for matrix exponentials

Classical Mechanics

Newton's Law of motion:

$$\sum f = m \ddot{x}$$

Lagrange Equations:

$$\frac{d}{dt}\left(\frac{\partial l}{\partial \dot{x}}\right) - \frac{\partial l}{\partial x} = 0 \quad , \qquad l = \frac{1}{2} m v^2 - V(x)$$

Hamilton has shown that the Lagrange equation is equivalent to this system of two partial differential equations:

$$\frac{\partial H}{\partial p_k} = \dot{q}_k \quad , \quad \frac{\partial H}{\partial q_k} = -\dot{p}_k \quad , \quad H = \sum_{m=1}^{k} \frac{1}{2} m \dot{q}_m^2 + V(q_1, q_2, \ldots, q_k)$$

$$p_k = m \dot{q}_k$$

Quantum Mechanics

In classical physics, $\boldsymbol{x}(\boldsymbol{t})$ is a function which describes the trajectory of the center of mass exactly, where In quantum mechanics $\boldsymbol{x}(\boldsymbol{t})$ is replaced by the wave function $\psi(\boldsymbol{x},\boldsymbol{t})$.

There will be no more classical functions and operators whose eigenvalues are the observable value take their places.

$$x \rightarrow \hat{x} \quad , \quad p \rightarrow -i\hbar\nabla \quad , \quad E \rightarrow i\hbar\partial_t$$

As it is seen in the formulas above there is a correlation between **Position-Momentum** and **Energy-Time.**

Using the transformations above and placing them into Hamilton's Equation will lead us to one of the most important Equations of Quantum Mechanics, The Schrödinger Equation.

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

Quantum Mechanics

As it is seen in the last slide the normal functions like $V(x)$ have been changed into $\hat{V}(x)$, which shows that they are Quantum operators.

As said before there will be a correlation between some operators in Quantum, when changing into Quantum Mechanics we will be dealing with probabilities not exact values, and the Heisenberg's uncertainty relations show us how exact we can be and at what costs.

$$\Delta x \Delta p \geqslant \hbar \quad , \quad \Delta E \Delta t \geqslant \hbar$$

This means if we want more accuracy in Position then we will lose accuracy in Momentum and vise versa.
The same goes for Energy Time but with slightly different interpretation (depending on the experiment) while the second one is derived from experiments and the first from Theory.

Spin

Spin is where Relativity steps into Quantum Mechanics, Spin is often said to be the **rest Angular Momentum**, it is not angular momentum but it has the same characteristics and since the electron even at rest has this attribute most of the Physicist don't like to call it Angular Momentum (Momentum means movement).

But when you solve the Schrödinger Equation (If the potential is analytically solvable) you won't result in spin cause the Schrödinger Equation is a non-relativistic equation. Nevertheless physicists just add the spin part to the wave function by hand. To derive the spin from formulas one needs to switch to Dirac's equation.

Spin was found in 1922, when Otto Stern and Walther Gerlach experimented with accelerated atoms in inhomogeneous magnetic fields, and saw that the rays split into two parts. Which was due to their spin.

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) $<\uparrow|$, $<\downarrow|$
Therefore we can write the spin state of our electron as a complex linear combination of these two vectors

$$\begin{pmatrix}\alpha\\ \beta\end{pmatrix} = \alpha <\uparrow| + \beta <\downarrow| \quad \in \mathbb{C}$$

Because $|\alpha|^2$ equals the probability of finding $|\uparrow>$ in an experiment and $|\beta|^2$ equals the probability of finding $|\downarrow>$, the normalization condition is

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

Spin

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:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_y = \begin{pmatrix} 0 & -i \\ -i & 0 \end{pmatrix} \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad , \quad \hat{S}_i = \frac{\hbar}{2} \sigma_i$$

Spin Coupling

The Kronecker tensor-product

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:

$$<\uparrow| \otimes <\downarrow| =: <\uparrow\downarrow|$$

$$<\uparrow| \otimes <\uparrow| =: <\uparrow\uparrow|$$

$$<\downarrow| \otimes <\downarrow| =: <\downarrow\downarrow|$$

$$<\downarrow| \otimes <\uparrow| =: <\downarrow\uparrow|$$

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

Spin Coupling

The potential between two spins is direct proportional to the scalar product of the two spin operators or to be more exactly their eigenvalues:

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

With μ being a constant and $\hat{S}_\pm = \hat{S}_x \pm i \hat{S}_y$ being the Ladder Operators.

$$\hat{S}_+ |\uparrow> = 0 \qquad \hat{S}_+ |\downarrow> = \hbar |\uparrow>$$

$$\hat{S}_- |\uparrow> = \hbar |\downarrow> \qquad \hat{S}_- |\downarrow> = 0$$

NMR

Nuclear Magnetic Resonance (NMR) is a physical phenomenon based upon the Quantum Mechanical magnetic properties of an atom's Nucleus. NMR also commonly refers to a family of scientific methods that exploit Nuclear Magnetic Resonance to study molecules.

All Nuclei that contain odd numbers of Protons or Neutrons have an intrinsic magnetic moment and Angular Momentum.

Credit: Wikipedia

NMR

As said before the Schrödinger Equation gives us the solutions to Quantum problems:

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

In NMR the particles don't move so we won't need the $\frac{-\hbar^2}{2\mathrm{m}}\nabla$ term Which is the Momentum part.

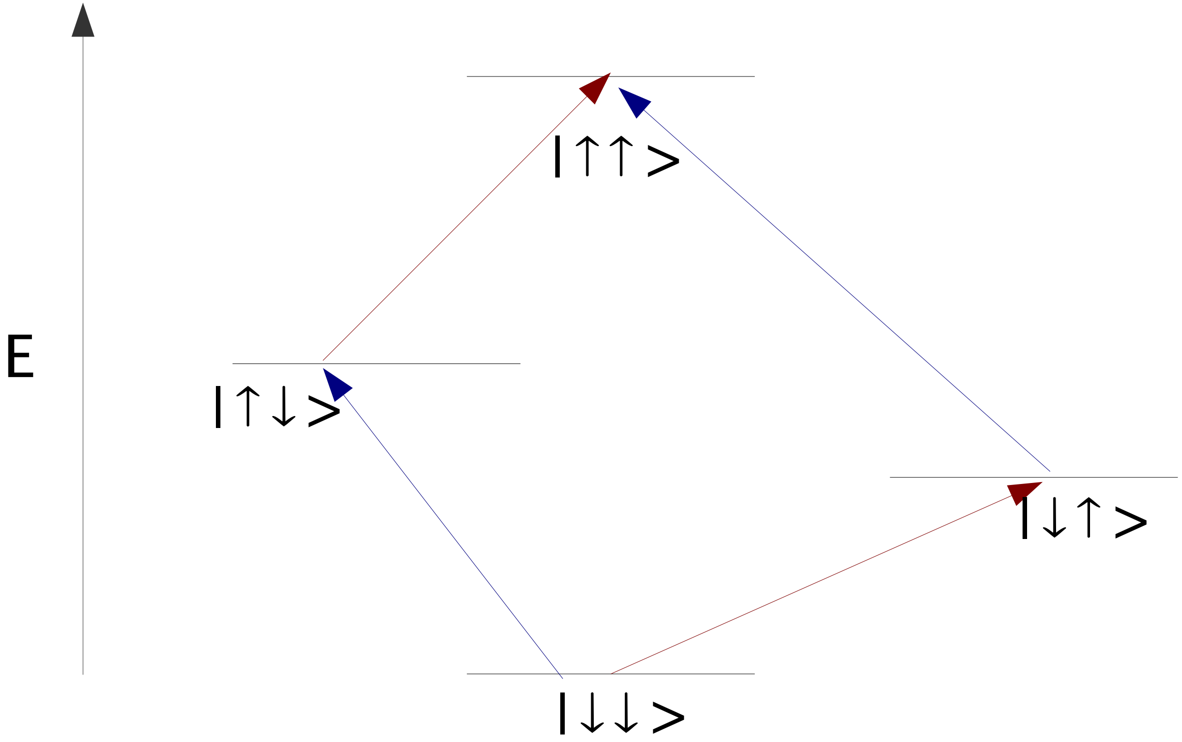
Furthermore we need to construct the Potential Operator, for that we already know the Potential between 2 particles and we can construct the Potential Operator as follows:

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

This is a $2^n\times 2^n$ Matrix which can be diagonalized and we will refer to it as H_d

Control Term

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.



Induced spin flips in a two particle system: red is due to $1_2 \otimes \hat{S}_+$ and blue is due to $\hat{S}_+ \otimes 1_2$

Control Term

For more than 2 spins the general formula will look like:

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

which is the control part and we will call it H_c

An easier way to construct the H_c is to use the recursion formula below

$$A_{n+1} = \begin{pmatrix} A_n & 1_{2^n} \\ 1_{2^n} & A_n \end{pmatrix} \qquad A_0 = 0$$

Matrix Exponential

Assuming that the solution to the Schrödinger Equation at time $t=0$ to be $\psi(0)$ the solution to the Schrödinger Equation at time t will be derived as follows:

$$\psi(t)=e^{-i\hat{H}t}\psi(0)$$

The exponential can be rewritten as

$$e^{-i\hat{H}t}=\sum_{k=0}^{\infty}\frac{(-i\hat{H}t)^k}{k!}$$

$$\hat{H}=H_d+H_c(u_1(t),u_2(t),....)=H_d+\Sigma_j H_j(t)$$

Where each $H_j(t)$ Operator is $e^{-i\hat{H}\Delta t}$

$$\psi(t)=e^{-i\hat{H}(t_k)\Delta t}e^{-i\hat{H}(t_{k-1})\Delta t}....e^{-i\hat{H}(t_1)\Delta t}\psi(0)=:u(t)\psi(0)=\psi(t),$$

$$k\Delta t=t$$

Matrix Exponential

Quantum Gate

A quantum gate is an operation on the spin state of the system which performs a desired change in it, for example : 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 maximizing the real part of $tr(u_G^t u(t))$

where $\partial_t u(t) = -i\hat{H} u(t)$ optimizes the propagator.

The GRAPE Algorithm

1) Set initial controls $u_j^{(r)}(t_k)$ for all times t_k at random or by guess

2)For each $k\in\{1,2,.\ldots.,M-1,M\}$ do:

2.1)Calculate the forward-propagation

$$u(t_k)=e^{-i\Delta\hat{H}(t_k)}e^{-i\Delta\hat{H}(t_{k-1})}\ldots e^{-i\Delta\hat{H}(t_1)}$$

2.2)Calculate the backward-propagation

$$\Lambda(t_k)=e^{-i\Delta\hat{H}(t_k)}e^{-i\Delta\hat{H}(t_{k+1})}\ldots e^{-i\Delta\hat{H}(t_M)}$$

2.3)Update $u_j^{(r+1)}(t_k)=u_j^{(r)}(t_k)+\epsilon\Re(tr(\Lambda^t(t_k)(-i\hat{H}_j)u(t_k)))$

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

Challenges of the GRAPE Algorithm

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 although this cannot be proven.

One has to calculate the exponential of a sparse matrix

$$u_k := e^{-i \Delta t \hat{H}(t_k)}$$

One has to calculate the product of many different matrices

$$u(t_k) = u_k . u_{k-1} ..... u_1$$

One has to calculate the trace

$$tr\{(u_k u_{k+1} .... u_m)(-i \hat{H}_j)(u_k u_{k-1} ... u_1)\}$$

Algorithms for matrix exponentials

As we saw in the GRAPE Algorithm we need to calculate Matrix Exponential and the problem is that we need to calculate all intermediate matrices

So we need to find some ways to do this part fast enough.

Ideas might be:
1) Diagonalize A (Eigendecomposition)
2) Approximate the exponential function
   i) with polynomials
      a) TAYLOR series
      b) CHEBYSHEV series expansion
   ii) with rational functions
      PADE approximation

Algorithms for Matrix Exponential

Eigendecomposition

A Diagonal matrix exponential is trivial

$$A = diag(d_1, d_{2,} \ldots., d_n)$$

$$e^A = diag(e^{d_1}, e^{d_2}, \ldots, e^{d_n})$$

And if $H = SDS^{-1}$ then we can calculate the exponential in the following way.

$$e^A = S(diag(e^{d_1}, \ldots., e^{d_n}))S^{-1}$$

But eigendecomposition is expensive.

Algorithms for Matrix Exponential

Taylor Series

We cam use partial sum of the Taylor series

$$e^A \approx S_m(A) := \sum_{k=0}^{m} \frac{A^k}{k!}$$

The error estimate depends on the norm of A.
Scaling & Squaring

Convergence is slow.

Not numerically stable.

Algorithms for Matrix Exponential

Chebychev polynomials

A well-behaved function $f:[-1,1]\rightarrow\mathbb{C}$ can be approximated by Chebychev polynomials $T_k(x)$

$$f(x)\approx\frac{a_0}{2}+\sum_{k=1}^{m} a_k T_k(x)$$

$$a_k:=\frac{2}{\pi}\int_{-1}^{1} f(x)T_k(x)\frac{dx}{\sqrt{1-x^2}}$$

For the exponential function, a_k decreases as $\dfrac{1}{2^k k!}$

This works also for matrices if the norm is smaller than one

Arbitrary norm: scaling & Squaring

Algorithms for Matrix Exponential

Pade approximation

Pade approximation works like Taylor, but using a rational function instead of a polynomial

For $x \in \mathbb{C}$ the Pade approximation $r_m(x)$ of e^x is given by

$$r_m(x) = \frac{p_m(x)}{q_m(x)}$$

$$p_m(x) = \sum_{j=0}^{m} \frac{(2\mathrm{m}-j)!\,m!}{(2\mathrm{m})!\,(m-j)!\,j!} x^j ,$$

$$q_m(x) = \sum_{j=0}^{m} \frac{(2\mathrm{m}-j)!\,m!\,(-1)^j}{(2\mathrm{m})!\,(m-j)!\,j!} x^j$$

Approximation is only good around 0

We need to compute the matrix inverse

Advantages of the Chebyshev series method

Only the evaluation of a matrix polynomial required

Only products of the form dense sparse appear

Good convergence properties

Matrix polynomials of order k can be evaluated with only $O(\sqrt{k})$ matrix–matrix–products

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Thank You