Making sense of sensing?

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Motivation and Content

These notes aim at linking entanglement in quantum mechanical systems with quantum sensing using simple examples. Numerical codes are included in order to illustrate basic elements of sensing. The examples are tailored to simple one- and two-qubit systems. The material contains (as of now, March 14, 2025))

1. One-qubit system with basic elements of sensing
2. Linking analytically solvable case with many-qubit entanglement and sensing
3. Simple two-particle (or two-qubit) system to demonstrate entanglement and its links with sensing (to come)
4. Numerical codes for simple time-dependent interactions

More material will be added

In particular, we will include

- ▶ Quantum computing simulations of the above systems using the Variational Quantum Eigensolver algorithm
- ▶ Discussion of Fisher entropy and other measures
- ▶ Numerical codes for general time-dependent interactions
- ▶ Initial state preparations and final results and more

Feel free to come with suggestions for additions. You can access the material as a jupyter-notebook at `https://github.com/mhjensenseminars/MachineLearningTalk/blob/master/doc/pub/sensing/ipynb/sensing.ipynb` or as a PDF file at `https://github.com/mhjensenseminars/MachineLearningTalk/blob/master/doc/pub/sensing/pdf/sensing.pdf`

Literature

In the discussions here we have borrowed extensively from two Review of Modern Physics articles

1. **Quantum sensing**, C.L. Degen, F. Reinhard, and P. Cappellaro, Reviews of Modern Physics **89**, 035002 (2017), see https://journals.aps.org/rmp/abstract/10.1103/RevModPhys.89.035002

2. **Quantum metrology with nonclassical states of atomic ensembles**, L. Pezzè, A. Smerzi, M.K. Oberthaler, R. Schmied, and P. Treutlein, Reviews of Modern Physics **90**, 035005 (2018), see https://journals.aps.org/rmp/abstract/10.1103/RevModPhys.90.035005

3. See also recent work by Liu et at https://www.nature.com/articles/s41534-021-00507-x. We may add codes which simulate these systems as well, stay tuned.

One-qubit system

In the first part of this notebook, we will analyze our systems using plain diagonalization and simple analytical manipulations.

Thereafter we will develop codes and material for performing a quantum computing simulation of the same systems (this material is not yet ready).

Our first encounter is a simple one-qubit system, described by a simple 2×2 Hamiltonian.

We start with a simple 2×2 Hamiltonian matrix expressed in terms of Pauli X, Y and Z matrices. But before we proceed, a simple reminder is appropriate.

Definitions: Single qubit gates

The Pauli matrices (and gate operations following therefrom) are defined as

$$\boldsymbol{X} \equiv \sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \boldsymbol{Y} \equiv \sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad \boldsymbol{Z} \equiv \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}.$$

Pauli-X gate

The Pauli-X gate is also known as the **NOT** gate, which flips the state of the qubit.

$$X|0\rangle = |1\rangle,$$
$$X|1\rangle = |0\rangle.$$

The Pauli-Y gate flips the bit and multiplies the phase by i.

$$Y|0\rangle = i|1\rangle,$$
$$Y|1\rangle = -i|0\rangle.$$

The Pauli-Z gate multiplies only the phase of $|1\rangle$ by -1.

$$Z|0\rangle = |0\rangle,$$
$$Z|1\rangle = -|1\rangle.$$

Hadamard gate

The Hadamard gate is defined as

$$\boldsymbol{H} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}.$$

It creates a superposition of the $|0\rangle$ and $|1\rangle$ states.

$$\boldsymbol{H}|0\rangle = \frac{1}{\sqrt{2}} \left(|0\rangle + |1\rangle \right), \tag{1}$$

$$\boldsymbol{H}|1\rangle = \frac{1}{\sqrt{2}} \left(|0\rangle - |1\rangle \right). \tag{2}$$

Note that we will use H as symbol for the Hadamard gate while we will reserve the notation $\mathcal{H}$ for a given Hamiltonian.

Sensing Hamiltonian

For our discussions, we will assume that the quantum sensor can be described by the generic Hamiltonian (we follow here Degen *et al.*,)

$$\mathcal{H}(t) = \mathcal{H}_0 + \mathcal{H}_I(t) + \mathcal{H}_{\mathrm{control}}(t),$$

where $\mathcal{H}_0$ is the internal Hamiltonian, $\mathcal{H}_I(t)$ is the Hamiltonian associated with a signal ($V(t)$ in the notes below), and $\mathcal{H}_{\mathrm{control}}(t)$ is the control Hamiltonian. Following the above mentioned authors, we will assume that $\mathcal{H}_0$ is known and that $\mathcal{H}_{\mathrm{control}}(t)$ can be chosen so as to manipulate or tune the sensor in a controlled way. The goal of a quantum sensing experiment is then to infer $V(t)$ from the effect it has on the actual qubits via its Hamiltonian $\mathcal{H}_I(t)$, usually by a specific choice of $\mathcal{H}_{\mathrm{control}}(t)$.

Time-dependent Hamiltonian matrix

We define a hermitian matrix $\mathcal{H} \in \mathbb{C}^{2\times 2}$

$$\mathcal{H} = \begin{bmatrix} \mathcal{H}_{11} & \mathcal{H}_{12} \\ \mathcal{H}_{21} & \mathcal{H}_{22} \end{bmatrix}.$$

We let $\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_I$, where

$$\mathcal{H}_0 = \begin{bmatrix} E_0 & 0 \\ 0 & E_1 \end{bmatrix},$$

is a diagonal matrix. Similarly,

$$\mathcal{H}_I(t) = \begin{bmatrix} V_{11}(t) & V_{12}(t) \\ V_{21}(t) & V_{22}(t) \end{bmatrix},$$

where $V_{ij}(t)$ represent various time-dependent interaction matrix elements and since we have a hermitian matrix, we require that $V_{21} = V_{12}^*$.

Interaction part

We will now label the interaction matrix elements, assuming that they have an explicit time dependence. We define

$$V_{11} = V_z(t)$$
$$V_{22} = -V_z(t)$$
$$V_{12} = V_x(t) - \imath V_y(t).$$

In the numerical example below we let $V_y(t) = 0$, $V_z(t) = tV_z$ and $V_x(t) = tV_x$ with V_z and V_x being real-valued constants to be determined. In the same numerical example we let $t \in [0, 1]$.

Non-interacting solution

We can view $\mathcal{H}_0$ as the non-interacting solution

$$\mathcal{H}_0|0\rangle = E_0|0\rangle,$$

and

$$\mathcal{H}_0|1\rangle = E_1|1\rangle,$$

where we have defined the orthogonal computational one-qubit basis states $|0\rangle$ and $|1\rangle$.

Rewriting with Pauli matrices

We rewrite $\mathcal{H}$ (and $\mathcal{H}_0$ and $\mathcal{H}_I$) via Pauli matrices

$$\mathcal{H}_0 = \mathcal{E}_{\mathrm{avg}}I - \Delta E\,\boldsymbol{Z}, \quad \mathcal{E}_{\mathrm{avg}} = \frac{E_0 + E_1}{2}, \; \Delta E = \frac{E_1 - E_0}{2},$$

and

$$\mathcal{H}_I = V_z(t)\boldsymbol{Z} + V_x(t)\boldsymbol{X} + V_y(t)\boldsymbol{Y},$$

with $V_z(t) = V_{11} = -V_{22}$, $V_x(t) = \Re(V_{12})$ and $V_y(t) = \Im(V_{12})$. This is the expression we will discuss in connection with quantum computing simulations. The discussions here, focus mainly on some simpler analytical considerations and simplifications. The numerical solutions are also given by standard eigenvalue solvers.

Simple time dependence

We let our Hamiltonian depend linearly on time t

$$\mathcal{H} = \mathcal{H}_0 + t\mathcal{H}_\mathrm{I},$$

with $t \in [0, 1]$, where the limits $t = 0$ and $t = 1$ represent the non-interacting (or unperturbed) and fully interacting system, respectively. This means that the various potential terms are given by $V_i(t) = tV_i$, with $i = \{x, y, z\}$ and V_i are real-valued constants.

Exact solution

Since this a simple 2×2 matrix eigenvalue problem we find the eigenvalues λ_0 and λ_1 to be

$$\lambda_{0,1} = \mathcal{E}_{\mathrm{avg}} \pm \Delta E \sqrt{1 + \frac{2V_z(t)}{\Delta E} + \frac{1}{\Delta E^2}(V_z^2(t) + V_x^2(t) + V_y^2(t))}.$$

If we assume that $\Delta E \gg V_z(t)$ and set $V_x(t) = V_y(t) = 0$ for simplicity and Taylor-expand our square root expression, we obtain

$$\lambda_0 = E_0 - \frac{1}{2}V_z(t),$$

$$\lambda_1 = E_1 + \frac{1}{2}V_z(t),$$

where we kept only terms up to ΔE. The above problem can however be easily solved numerically, see the code here.

Selecting parameters

The model is an eigenvalue problem with only two available states. Here we set the parameters $E_0 = 0$, $E_1 = 4$, $V_{11} = -V_{22} = 3$ and $V_{12} = V_{21} = 0.2$.

The non-interacting solutions represent our computational basis. Pertinent to our choice of parameters, is that at $t \geq 2/3$, the lowest eigenstate is dominated by $|1\rangle$ while the upper is $|0\rangle$. At $t = 1$ the $|0\rangle$ mixing of the lowest eigenvalue is 1% while for $t \leq 2/3$ we have a $|0\rangle$ component of more than 90%. The character of the eigenvectors has therefore been interchanged when passing $z = 2/3$. The value of the parameter V_{12} represents the strength of the coupling between the two states. Here we keep only the real part of the non-diagonal term.

Setting up the matrix for the simple one-qubit system

Here we solve the above problem as a standard eigenvalue problem (best seen using the jupyter-notebook)

```python
import numpy as np
import matplotlib.pyplot as plt
import seaborn as sns; sns.set_theme(font_scale=1.5)
from tqdm import tqdm

sigma_x = np.array([[0, 1], [1, 0]])
sigma_y = np.array([[0, -1j], [1j, 0]])
sigma_z = np.array([[1, 0], [0, -1]])
I = np.eye(2)

def Hamiltonian(lmb):
    E0 = 0
    E1 = 4
    V11 = 3
    V22 = -3
    V12 = 0.2
    V21 = 0.2

    eps = (E0 + E1) / 2
    omega = (E0 - E1) / 2
    c = (V11 + V22) / 2
    omega_z = (V11 - V22) / 2
    omega_x = V12

    H0 = eps * I + omega * sigma_z
```

Sensing protocol, taken from Degen *et al.,*

1. The quantum sensor is initialized in some known basis, say $|0\rangle$.

2. The quantum sensor is transformed into the desired inittial state $|\psi_{\text{Initial}}\rangle$, through an appropriate transformation $\boldsymbol{U}_1$. For a single qubit system this could be a Hadamard gate which results in a linear superposition of $|0\rangle$ and $|1\rangle$.

3. The quantum sensor evolves under the Hamiltonian $\mathcal{H}$ for a time t. At the end of the sensing period, the sensor is in its final stage (see below) $|\psi(t)\rangle = \boldsymbol{U}_{\mathcal{H}}(t,0)|\psi_{\text{Initial}}\rangle$

4. This quantum state is transformed into a superposition of observable readout states, say a superposition of the one=qubit states $|0\rangle$ and $|1\rangle$, via the action $\boldsymbol{U}_2|\psi(t)\rangle$.

5. The final state of the quantum sensor is read out.

6. Steps 1-5 are repeated and averaged over a large number of cycles N to estimate the final transition probabilities p.

7. The transition probability p is measured as a function of time t and used to infer to desired signal $V(t)$.

We stay now with the Taylor-approximated solution from the simple example above (the one-qubit case). We do so in order to illustrate some of the basic sensing ideas.

To initialize a given system to a known quantum state, we first start with a known initial state $|0\rangle$. Then, depending on the type of information that we want to learn about the stimulus, the measurement scheme to be used, and the physical implementation of the quantum system, we choose some unitary operator $\boldsymbol{U}_{\text{Initial}}$ such that it transforms our state $|0\rangle$ to a desired initial superposition state $|\psi_{\text{Initial}}\rangle = a|0\rangle + b|1\rangle$ for some $a, b \in \mathbb{C}$ such that $|a|^2 + |b|^2 = 1$.

Effects of stimulus

After the sensing state is initialized, it is exposed to the environment and evolves according to the time-evolution operator of the sensing Hamiltonian via the unitary transformation $\boldsymbol{U}_{\mathcal{H}}$ as (setting $\hbar = c = e = 1$)

$$|\psi(t)\rangle = \boldsymbol{U}_{\mathcal{H}}(t, 0) |\psi_{\text{Initial}}\rangle.$$

In general we have

$$\boldsymbol{U}_{\mathcal{H}} = \exp\left(\imath \int_0^t \mathcal{H}(\tau)d\tau\right).$$

Here the Hamiltonian could be a complicated, non-analytical function with a time-dependent $V(t)$ (making $\mathcal{H}$ time-dependent as well).

Slowly changing potential

In the case where $V(t)$ is constant or changes much more slowly than our sensing integration time, we can assume

$$|\psi(t)\rangle = \boldsymbol{U}_{\mathcal{H}}(t, 0) |\psi_{\text{Initial}}\rangle = \exp\left(\imath t \mathcal{H}\right) |\psi_{\text{Initial}}\rangle.$$

The sensing state evolves thus as

$$|\psi(t)\rangle = \left(\exp \imath t \left(E_0 - \frac{1}{2} V_z\right) |\lambda_0\rangle \langle\lambda_0| + \exp \imath t \left(E_1 + \frac{1}{2} V_z\right) |\lambda_1\rangle \langle\lambda_1|\right) |$$

where we have using the spectral decomposition and the final representation of the sensing Hamiltonian found above.

Readout

After the sensing state has evolved over time in the presence of $V(t)$, it can be transformed again before a measurement is taken. The first part, the transformation to some desired read-out state, is performed by a readout operator, see discussions in Degen et al., 2017) where

$$|\psi_{\mathrm{Final}}\rangle = \boldsymbol{U}_{\mathrm{Readout}}|\psi(t)\rangle.$$

Here the readout operator $\boldsymbol{U}_{\mathrm{Readout}}$ is left unspecified.

Measurement

A measurement of this final state $|\psi_{\text{Final}}\rangle = a'|0\rangle + b'|1\rangle$ is made with respect to the basis $\{|0\rangle, |1\rangle\}$ where $|0\rangle$ is measured with probability

$$|\langle 0 \mid \psi_{\text{Final}}\rangle|^2 = \left|a'\right|^2,$$

and $|1\rangle$ is measured with probability

$$|\langle 1 \mid \psi_{\text{Final}}\rangle|^2 = \left|b'\right|^2.$$

After this measurement, the sensing state has collapsed into one of the basis states and no more information can be gained.

Multiple measurements

However, by having multiple quantum sensing elements time-evolving together or by repeating the process many times before the external stimulus $V(t)$ can change, a transition probability

$$p_{|0\rangle \to |1\rangle} = |\langle 1 \mid \psi_{\mathrm{Final}}\rangle|^2 = \left|b'\right|^2,$$

can be estimated. The *sensing* is then achieved by taking a series of these transition probabilities as a time series, and then using the results to estimate the sensed stimulus $V(t)$, see for example the abovementioned review of Degen et al., 2017.

Example

The simplest mathematical example of quantum sensing is sensing an external stimulus's effect on the splitting of the energy levels of an isolated system. Suppose our stimulus is constant and *parallel* with our sensor, that is we set $V_z(t) = V_0$ and $V_x = 0$, and we choose our initialization and readout preparation operators to be the famous Hadamard gate

$$\boldsymbol{U}_H = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}.$$

Here, the subscript H stands for the Hadamard unitary transformation.

Evolution of initial state

The initial state is

$$|\psi_{\text{Initial}}\rangle = \boldsymbol{U}_H|0\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix}.$$

This may not necessarily be the same basis into which the system was initialized, but we assume it is so and then we only have to keep track of one basis.

State evolution

The state evolves as

$$|\psi(t)\rangle = \left(\exp \imath t \left(E_0 - \frac{1}{2} V_z \right) |0\rangle\langle 0| + \exp \imath t \left(E_1 + \frac{1}{2} V_z \right) |1\rangle\langle 1| \right) |\psi_{\text{Initial}}\rangle$$

$$= \frac{1}{\sqrt{2}} \exp \imath t \left(E_0 - \frac{1}{2} V_z \right) \left[\begin{matrix} 1 \\ \exp \imath t \left(E_1 - E_0 + V_z \right) \end{matrix} \right]$$

Preparing for readout

This is then prepared for readout as

$$|\psi_{\text{Final}}\rangle = \frac{1}{2} \exp \imath t(E_0 - \frac{1}{2}V_z) \begin{bmatrix} 1 + \exp \imath t(E_1 - E_0 + V_z) \\ 1 - \exp \left(\imath t(E_1 - E_0 + V_z)\right) \end{bmatrix}.$$

Transition probability

The transition probability

$$p_{|0\rangle \to |1\rangle} = |\langle 1 \mid \psi_{\text{Final}}\rangle|^2 = |1 - \exp \imath t \left(E_1 - E_0 + V_z\right)|^2$$

$$= \frac{1}{2} \left(1 - \cos \left(t \left(E_1 - E_0\right) + V_z\right)\right)$$

Ramsey interferometry

We know the difference in energy between E_1 and E_0, either since we constructed the system or by taking measurements without the external stimulus V, and we can control the time t for which the system is allowed to evolve under the external stimulus. Then we can fix t and take many measurements to estimate $p_{|0\rangle \to |1\rangle}$, which then makes finding tV_z a simple phase-estimation problem which gives us V_z. The physical implementation of this process is known as Ramsey Interferometry, and it can be done with arbitary initialization and readout preparation unitary operators.

Up until now, we have said that we take many measurements of $|\psi_{\mathsf{Final}}\rangle$ to estimate $p_{|0\rangle \to |1\rangle}$, but we have neglected the estimation process. Assuming we can take N measurements, either by having N experimental apparatuses running in parallel or by taking N different measurements of a (relatively) constant V with a single apparatus (this is what we will do below), the uncertainty in p, denoted as σ_p (this is a positive real number; not to be confused with the Pauli matrices), scales as

$$\sigma_p \propto \frac{1}{\sqrt{N}}$$

Ramsey interferometry

If we consider Ramsey Interferometry as an example, see
https://en.wikipedia.org/wiki/Ramsey_interferometry,
then the uncertainty in V_z, denoted σ_V, scales as

$$\sigma_V \propto \sigma_p \propto \frac{1}{\sqrt{N}}$$

This relationship is known as the standard quantum limit (SQL) ,
see Giovannetti *et al.*, 2011,
https://www.nature.com/articles/nphoton.2011.35, but can
also be explained with the law of Large Numbers from statistics,
where measuring N similarly distributed, well-behaved random
variables gives the sample mean as an estimator for the population
mean and the sample variance divided by the size of the sample as
an uncertainty in the estimate of the population mean.

Key components of code for one qubit

Physical System:

1. Hamiltonian: $\mathcal{H} = -\frac{\gamma B}{2} Z$ (we will set $\gamma = 1$)
2. Initial state: $|\psi_{\text{Initial}}\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$, Hadamard gate

Time Evolution:

1. Calculated using matrix exponential: $U_{\mathcal{H}}(t) = \exp{-i\mathcal{H}t}$
2. State at time t: $|\psi(t)\rangle = U_{\mathcal{H}}(t)|\psi_{\text{Initial}}\rangle$

Expectation Values:

1. $\langle X \rangle$: Oscillates as $\cos(Bt)$
2. $\langle Y \rangle$: Oscillates as $-\sin(Bt)$
3. $\langle Z \rangle$: Remains constant at 0

One-qubit program example (best seen using the jupyter-notebook)

```python
import numpy as np
from scipy.linalg import expm
import matplotlib.pyplot as plt

# Define single-qubit operations, Identity, Pauli, Hadamard and S matr
Id = np.array([[1, 0], [0, 1]], dtype=complex)
X = np.array([[0, 1], [1, 0]], dtype=complex)
Y = np.array([[0, -1j], [1j, 0]], dtype=complex)
Z = np.array([[1, 0], [0, -1]], dtype=complex)
Had = np.array([[1, 1],[1, -1]], dtype=complex) / np.sqrt(2)
S = np.array([[1, 0],[0, 1j]], dtype=complex)

# Simulation parameters
B = 2 * np.pi   # Magnetic field strength (in angular frequency units)
times = np.linspace(0, 1, 200)   # Time range from 0 to 1 seconds

# Initial state: superposition state via Hadamard gate acting on |0>
psi0 = np.array([1, 0], dtype=complex) # start with |0> then act with
psi0 = Had @ psi0

# Lists to store expectation values
expect_x, expect_y, expect_z = [], [], []

for t in times:
    # Construct Hamiltonian
    H = B * Z/ 2
```

Interpretation

1. The oscillations in X and Y components demonstrate the Larmor precession caused by the magnetic field
2. The frequency of oscillation is directly proportional to the magnetic field strength B
3. This forms the basis for quantum sensing: measuring oscillation frequency allows precise determination of B

To use this for sensing (protocol of Degen *et al.*, (2017))

1. Prepare the qubit in a known superposition state
2. Let it evolve in the magnetic field for a known time
3. Measure the expectation values
4. Determine (here) B from the oscillation frequency

Feel free to play around with this code

1. Change *B* value to see different oscillation frequencies
2. Adjust *time* array to observe different numbers of oscillations
3. Add noise to simulate real-world sensing scenarios
4. Implement actual measurement simulations instead of expectation values

This code provides a fundamental demonstration of quantum sensing principles using a simple qubit system. Real-world implementations would typically use more sophisticated techniques like Ramsey interferometry or dynamical decoupling for enhanced sensitivity.

More than one qubit

The nature of quantum systems allows for more information to be extracted by exploiting entanglement between quantum systems. This is the fundamental basis for the benefits of quantum computing over classical computing, and quantum sensing has similar benefits over classical sensing. Suppose we return to the example above, but rather than initializing N sensing qubits separately, we initialize $\frac{N}{n}$ groups each with n entangled quantum systems. Then we have

$$|\psi_{\text{Init}}\,\rangle = \frac{1}{\sqrt{2^n}}\left(|0\rangle^{\otimes n} + |1\rangle^{\otimes n}\right),$$

where $|0\rangle^{\otimes n} = |0\rangle \otimes \ldots \otimes |0\rangle$, n times.

After initialization

After initialization, each of the n sensing qubits evolves to pick up a relative phase factor of $\exp \imath t \left(E_1 - E_0 + V_z \right)$, which combined results in

$$|\psi(t)\rangle = \mathcal{N} \left(|0\rangle^{\otimes n} + \exp n \imath t \left(E_1 - E_0 + V_z \right) |1\rangle^{\otimes n} \right)$$

where $\mathcal{N}$ is just a factor to take care of normalization.

Transition probability

The transition probability

$$p_{|0\rangle \to |1\rangle} = |\langle 1 \mid \psi_{\mathsf{Final}} \rangle|^2 = \frac{1}{2} \left(1 - \cos\left(tn\left(E_1 - E_0\right) + nV_z\right)\right)$$

Role of entanglement

From this, we can see that through entangling n sensing qubits, the **signal** we are trying to sense increases from $V_z \to nV_z$, and with $\frac{N}{n}$ total measurements,

$$\sigma_V \propto \frac{1}{n}\sigma_p \propto \frac{1}{n}\left(\frac{1}{\sqrt{\frac{N}{n}}}\right) = \frac{1}{\sqrt{Nn}}$$

which means the error decreased by a factor of $\sqrt{n}$. In the case where $n = N$, the uncertainty now scales as

$$\sigma_V \propto \frac{1}{N}$$

which is known as the Heisenberg limit, and is the quantum-mechanically limited, maximal amount of information one can get from taking n quantum sensing measurements, see again Giovannetti *et al.*, at
https://www.nature.com/articles/nphoton.2011.35.

Two qubits and entanglement

We will now look at a simple system where we can produce an entangled state. We focus on a two-qubit system.
Our computational basis states

$$|00\rangle = |0\rangle_A \otimes |0\rangle_B = \begin{bmatrix} 1 & 0 & 0 & 0 \end{bmatrix}^T,$$

and

$$|01\rangle = |0\rangle_A \otimes |1\rangle_B = \begin{bmatrix} 0 & 1 & 0 & 0 \end{bmatrix}^T,$$

and

$$|10\rangle = |1\rangle_A \otimes |0\rangle_B = \begin{bmatrix} 0 & 0 & 1 & 0 \end{bmatrix}^T,$$

and finally

$$|11\rangle = |1\rangle_A \otimes |1\rangle_B = \begin{bmatrix} 0 & 0 & 0 & 1 \end{bmatrix}^T.$$

Simple system to Illustrate entanglement

This system can be thought of as composed of two subsystems A and B. Each subsystem has computational basis states

$$|0\rangle_{A,B} = \begin{bmatrix} 1 & 0 \end{bmatrix}^T \qquad |1\rangle_{A,B} = \begin{bmatrix} 0 & 1 \end{bmatrix}^T.$$

The subsystems could represent single particles or composite many-particle systems of a given symmetry.

Computational basis states

This leads to the many-body computational basis states

$$|00\rangle = |0\rangle_A \otimes |0\rangle_B = \begin{bmatrix} 1 & 0 & 0 & 0 \end{bmatrix}^T,$$

and

$$|01\rangle = |0\rangle_A \otimes |1\rangle_B = \begin{bmatrix} 0 & 1 & 0 & 0 \end{bmatrix}^T,$$

and

$$|10\rangle = |1\rangle_A \otimes |0\rangle_B = \begin{bmatrix} 0 & 0 & 1 & 0 \end{bmatrix}^T,$$

and finally

$$|11\rangle = |1\rangle_A \otimes |1\rangle_B = \begin{bmatrix} 0 & 0 & 0 & 1 \end{bmatrix}^T.$$

Eigenstates of non-interacting Hamiltonian

These computational basis states define the eigenstates of the non-interacting Hamiltonian

$$H_0|00\rangle = \epsilon_{00}|00\rangle,$$

$$H_0|10\rangle = \epsilon_{10}|10\rangle,$$

$$H_0|01\rangle = \epsilon_{01}|01\rangle,$$

and

$$H_0|11\rangle = \epsilon_{11}|11\rangle.$$

Interaction part

The interacting part of the Hamiltonian H_I is given by the tensor product of two σ_x and σ_z matrices, respectively, that is

$$H_\mathrm{I} = H_x \sigma_x \otimes \sigma_x + H_z \sigma_z \otimes \sigma_z,$$

where H_x and H_z are interaction strength parameters. Our final Hamiltonian matrix is given by

$$\boldsymbol{H} = \begin{bmatrix} \epsilon_{00} + H_z & 0 & 0 & H_x \\ 0 & \epsilon_{10} - H_z & H_x & 0 \\ 0 & H_x & \epsilon_{01} - H_z & 0 \\ H_x & 0 & 0 & \epsilon_{11} + H_z \end{bmatrix}.$$

Entangled state

This system produces an initial state (we select the lowest-lying state) which is entangled (it acts like a SWAP gate) transforming the system from $|00\rangle$ at interaction strength 0 to

$$|\psi_{\text{Initial}}\rangle = \alpha|01\rangle + \beta|10\rangle.$$

We can then act with a given probe on this state and study its time-evolution, in the same way as we studied the one-qubit system. The code below (to be added) performs then

$$|\psi(t)\rangle = \boldsymbol{U}_{\mathcal{H}}(\alpha|01\rangle + \beta|10\rangle).$$
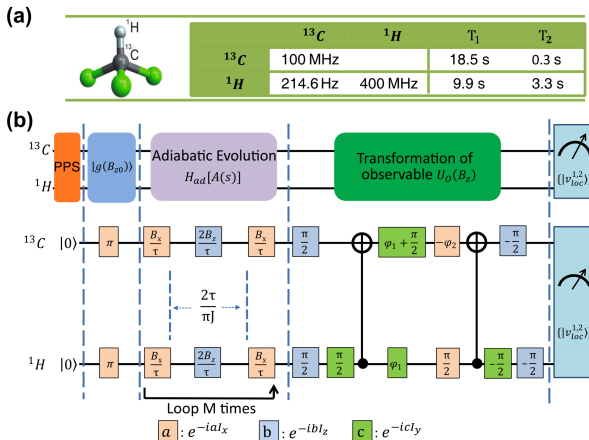
Sensing protocol and Gunnar's part

Fig. 2 Physical system and quantum circuit. a Molecular structure and relevant parameters of ^{13}C-labeled chloroform. **b** Experimental scheme and quantum circuit for the critical quantum metrology with adiabatic evolution on NMR. Here, $\varphi_1 = \arctan[(B_z - 1)/0] - \pi/4$, $\varphi_2 = |\theta - \pi/2|$, where $\theta = \sqrt{2}B_x/(1 - B_z)$. The specific pulse sequence for implementing in experiment can be seen in 'Methods' and Supplementary Note 4.

Intermezzo (digression) on density matrices and entropy

The four eigenstates of the above Hamiltonian matrix can in turn be used to define density matrices. As an example, the density matrix of the first eigenstate (lowest energy E_0) Ψ_0 is given by the outerproduct

$$\rho_0 = (\alpha_{00}|00\rangle + \alpha_{10}|10\rangle + \alpha_{01}|01\rangle + \alpha_{11}|11\rangle)(\alpha_{00}^*\langle 00| + \alpha_{10}^*\langle 10| + \alpha_{01}^*\langle 0$$

where the coefficients α_{ij} are the eigenvector coefficients resulting from the solution of the above eigenvalue problem.

Subsystems

We can then in turn define the density matrix for the subsets A or B as

$$\rho_A = \mathrm{Tr}_B(\rho_0) = \langle 0|\rho_0|0\rangle_B + \langle 1|\rho_0|1\rangle_B,$$

or

$$\rho_B = \mathrm{Tr}_A(\rho_0) = \langle 0|\rho_0|0\rangle_A + \langle 1|\rho_0|1\rangle_A.$$

Entropies

The density matrices for these subsets can be used to compute the so-called von Neumann entropy, which is one of the possible measures of entanglement. A pure state has entropy equal zero while entangled state have an entropy larger than zero. The von-Neumann entropy is defined as

$$S(A, B) = -\operatorname{Tr}\left(\rho_{A,B} \log_2(\rho_{A,B})\right).$$

Understanding the example

The example here shows the above von Neumann entropy based on the density matrix for the lowest many-body state. We see clearly a jump in the entropy around the point where we have a level crossing. At interaction strenght $\lambda = 0$ we have many-body states purely defined by their computational basis states. As we switch on the interaction strength, we obtain an increased degree of mixing and the entropy increases till we reach the level crossing point where we see an additional and sudden increase in entropy. Similar behaviors are observed for the other states. The most important result from this example is that entanglement is driven by the Hamiltonian itself and the strength of the interaction matrix elements and the non-interacting energies.

Code, best seen in jupyter-notebook

```python
%matplotlib inline
from  matplotlib import pyplot as plt
import numpy as np
from scipy.linalg import logm, expm
def log2M(a): # base 2 matrix logarithm
    return logm(a)/np.log(2.0)

dim = 4
Hamiltonian = np.zeros((dim,dim))
#number of lambda values
n = 40
lmbd = np.linspace(0.0,1.0,n)
Hx = 2.0
Hz = 3.0
# Non-diagonal part as sigma_x tensor product with sigma_x
sx = np.matrix([[0,1],[1,0]])
sx2 = Hx*np.kron(sx, sx)
# Diagonal part as sigma_z tensor product with sigma_z
sz = np.matrix([[1,0],[0,-1]])
sz2 = Hz*np.kron(sz, sz)
noninteracting = [0.0, 2.5, 6.5, 7.0]
D = np.diag(noninteracting)
Eigenvalue = np.zeros((dim,n))
Entropy = np.zeros(n)

for i in range(n):
    Hamiltonian = lmbd[i]*(sx2+sz2)+D
    # diagonalize and obtain eigenvalues, not necessarily sorted
```

Role of entanglement

As seen from this example, our initial state (the lowest lying one) is an entangled state

$$|\psi_{\text{Initial}}\rangle = \alpha|01\rangle + \beta|10\rangle.$$

We can then act with a given probe on this state and study its time-evolution, in the same way as we studied the one-qubit system. The code below) performs then

$$|\psi(t)\rangle = \boldsymbol{U}_{\mathcal{H}}(\alpha|01\rangle + \beta|10\rangle).$$

Thereafter we implement an explicit measurement. Note that this code does not compute these expectation values as one would when implementing a quantum computing approach. The subsequent example mimics the way we would run this as a real experiment.