January 22-26,2024: Measurements, spectral decomposition and Hamiltonians

Morten Hjorth-Jensen[1,2]

Department of Physics, University of Oslo, Norway[1]

Department of Physics and Astronomy and Facility for Rare Isotope Beams, Michigan State University, USA[2]

Jan 21, 2024

Summary from last week and plans for this week

Last week we:

1. defined the state vector and the associated notation
2. introduced the inner product and showed how to calculate it in an orthonormal basis
3. introduced outer products and projection operators
4. introduced tensor products and showed how to contruct state vectors for multiple qubits

This week's plans

We will repeat some of these topics today and discuss also

1. tensor products of Hilbert Spaces and definition of Computational Basis, partly repetition from last week
2. the idea of wavefunction collapse as a result of measurement
3. Spectral Decomposition, Measurements and Density matrices
4. Simple Hamiltonians and other operators
5. First exercise set and discussions of coding examples

- **Reading recommendation**: Scherer, Mathematics of Quantum Computations, chapter 3.1-3.3 and Hundt, Quantum Computing for Programmers, chapter 2.1-2.5. Hundt's text is relevant for the programming part where we build from scratch the ingredients we will need.

Measurements

The probability of a measurement on a quantum system giving a certain result is determined by the weight of the relevant basis state in the state vector. After the measurement, the system is in a state that corresponds to the result of the measurement. The operators and gates discussed below are examples of operations we can perform on specific states.
We consider the state

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$$

Properties of a measurement

1. A measurement can yield only one of the above states, either $|0\rangle$ or $|1\rangle$.
2. The probability of a measurement resulting in $|0\rangle$ is $\alpha^*\alpha = |\alpha|^2$.
3. The probability of a measurement resulting in $|1\rangle$ is $\beta^*\beta = |\beta|^2$.
4. And we note that the sum of the outcomes gives $\alpha^*\alpha + \beta^*\beta = 1$ since the two states are normalized.

After the measurement, the state of the system is the state associated with the result of the measurement.
We have already encountered the projection operators P and Q.
Let us now look at other types of operations we can make on qubit states.

Entanglement

In order to study entanglement and why it is so important for quantum computing, we need to introduce some basic measures and useful quantities. These quantities are the spectral decomposition of hermitian operators, how these are then used to define measurements and how we can define so-called density operators (matrices). These are all quantities which will become very useful when we discuss entanglement and in particular how to quantify it. In order to define these quantities we need first to remind ourselves about some basic linear algebra properties of hermitian operators and matrices.

Basic properties of hermitian operators

The operators we typically encounter in quantum mechanical studies are

1. Hermitian (self-adjoint) meaning that for example the elements of a Hermitian matrix $\boldsymbol{U}$ obey $u_{ij} = u_{ji}^*$.
2. Unitary $\boldsymbol{U}\boldsymbol{U}^\dagger = \boldsymbol{U}^\dagger\boldsymbol{U} = \boldsymbol{I}$, where $\boldsymbol{I}$ is the unit matrix
3. The oparator $\boldsymbol{U}$ and its self-adjoint commute (often labeled as normal operators), that is $[\boldsymbol{U}, \boldsymbol{U}^\dagger] = 0$. An operator is **normal** if and only if it is diagonalizable. A Hermitian operator is normal.

Unitary operators in a Hilbert space preserve the norm and orthogonality. If $\boldsymbol{U}$ is a unitary operator acting on a state $|\psi_j\rangle$, the action of

$$|\phi_i\rangle = \boldsymbol{U}|\psi_j\rangle,$$

preserves both the norm and orthogonality, that is $\langle\phi_i|\phi_j\rangle = \langle\psi_i|\psi_j\rangle = \delta_{ij}$, as discussed earlier.

The Pauli matrices again

As example, consider the Pauli matrix σ_x. We have already seen that this matrix is a unitary matrix. Consider then an orthogonal and normalized basis $|0\rangle^\dagger = \begin{bmatrix}1&0\end{bmatrix}$ and $|1\rangle^\dagger = \begin{bmatrix}0&1\end{bmatrix}$ and a state which is a linear superposition of these two basis states

$$|\psi_a\rangle = \alpha_0|0\rangle + \alpha_1|1\rangle.$$

A new state $|\psi_b\rangle$ is given by

$$|\psi_b\rangle = \sigma_x|\psi_a\rangle = \alpha_0|1\rangle + \alpha_1|0\rangle.$$

Spectral Decomposition

An important technicality which we will use in the discussion of density matrices, entanglement, quantum entropies and other properties is the so-called spectral decomposition of an operator. Let $|\psi\rangle$ be a vector in a Hilbert space of dimension n and a hermitian operator $\boldsymbol{A}$ defined in this space. Assume $|\psi\rangle$ is an eigenvector of $\boldsymbol{A}$ with eigenvalue λ, that is

$$\boldsymbol{A}|\psi\rangle = \lambda|\psi\rangle = \lambda \boldsymbol{I}|\psi\rangle,$$

where we used $\boldsymbol{I}|\psi\rangle = 1|\psi\rangle$. Subtracting the right hand side from the left hand side gives

$$[\boldsymbol{A} - \lambda \boldsymbol{I}]\,|\psi\rangle = 0,$$

which has a nontrivial solution only if the determinant $\det(\boldsymbol{A} - \lambda \boldsymbol{I}) = 0$.

ONB again and again

We define now an orthonormal basis $|i\rangle = \{|0\rangle, |1\rangle, \ldots, |n-1\rangle$ in the same Hilbert space. We will assume that this basis is an eigenbasis of $\boldsymbol{A}$ with eigenvalues λ_i
We expand a new vector using this eigenbasis of $\boldsymbol{A}$

$$|\psi\rangle = \sum_{i=0}^{n-1} \alpha_i |i\rangle,$$

with the normalization condition $\sum_{i=0}^{n-1} |\alpha_i|^2$. Acting with $\boldsymbol{A}$ on this new state results in

$$\boldsymbol{A}|\psi\rangle = \sum_{i=0}^{n-1} \alpha_i \boldsymbol{A}|i\rangle = \sum_{i=0}^{n-1} \alpha_i \lambda_i |i\rangle.$$

Projection operators

If we then use that the outer product of any state with itself defines a projection operator we have the projection operators

$$\boldsymbol{P}_{\psi} = |\psi\rangle\langle\psi|,$$

and

$$\boldsymbol{P}_{j} = |j\rangle\langle j|,$$

we have that

$$\boldsymbol{P}_{j}|\psi\rangle = |j\rangle\langle j| \sum_{i=0}^{n-1} \alpha_i |i\rangle = \sum_{i=0}^{n-1} \alpha_i |j\rangle\langle j|i\rangle.$$

Further manipulations

This results in

$$\boldsymbol{P}_j|\psi\rangle = \alpha_j|j\rangle,$$

since $\langle j|i\rangle$. With the last equation we can rewrite

$$\boldsymbol{A}|\psi\rangle = \sum_{i=0}^{n-1} \alpha_i \lambda_i |i\rangle = \sum_{i=0}^{n-1} \lambda_i \boldsymbol{P}_i|\psi\rangle,$$

from which we conclude that

$$\boldsymbol{A} = \sum_{i=0}^{n-1} \lambda_i \boldsymbol{P}_i.$$

Spectral decomposition

This is the spectral decomposition of a hermitian and normal operator. It is true for any state and it is independent of the basis. The spectral decomposition can in turn be used to exhaustively specify a measurement, as we will see in the next section.
As an example, consider two states $|\psi_a\rangle$ and $|\psi_b\rangle$ that are eigenstates of $\boldsymbol{A}$ with eigenvalues λ_a and λ_b, respectively. In the diagonalization process we have obtained the coefficients α_0, α_1, β_0 and β_1 using an expansion in terms of the orthogonal basis $|0\rangle$ and $|1\rangle$.

Explicit results

We have then

$$|\psi_a\rangle = \alpha_0|0\rangle + \alpha_1|1\rangle,$$

and

$$|\psi_b\rangle = \beta_0|0\rangle + \beta_1|1\rangle,$$

with corresponding projection operators

$$\boldsymbol{P}_a = |\psi_a\rangle\langle\psi_a| = \begin{bmatrix} |\alpha_0|^2 & \alpha_0\alpha_1^* \\ \alpha_1\alpha_0^* & |\alpha_1|^* \end{bmatrix},$$

and

$$\boldsymbol{P}_b = |\psi_b\rangle\langle\psi_b| = \begin{bmatrix} |\beta_0|^2 & \beta_0\beta_1^* \\ \beta_1\beta_0^* & |\beta_1|^* \end{bmatrix}.$$

The spectral decomposition

The results from the previous slide gives us the following spectral decomposition of $\boldsymbol{A}$

$$\boldsymbol{A} = \lambda_a |\psi_a\rangle\langle\psi_a| + \lambda_b |\psi_b\rangle\langle\psi_b|,$$

which written out in all its details reads

$$\boldsymbol{A} = \lambda_a \begin{bmatrix} |\alpha_0|^2 & \alpha_0\alpha_1^* \\ \alpha_1\alpha_0^* & |\alpha_1|^* \end{bmatrix} + \lambda_b \begin{bmatrix} |\beta_0|^2 & \beta_0\beta_1^* \\ \beta_1\beta_0^* & |\beta_1|^* \end{bmatrix}.$$

Measurements

Armed with the spectral decomposition, we are now ready to discuss how to compute measurements of observables. When we make a measurement, quantum mechanics postulates that mutually exclusive measurement outcomes correspond to orthogonal projection operators.
We assume now we can contruct a series of such orthogonal operators based on $|i\rangle \in \{|0\rangle, |1\rangle, \ldots, |n-1\rangle$ computational basis states. These projection operators $\boldsymbol{P}_0, \boldsymbol{P}_1, \ldots, \boldsymbol{P}_{n-1}$ are all idempotent and sum to one

$$\sum_{i=0}^{n-1} \boldsymbol{P}_i = \boldsymbol{I}.$$

Qubit example

As an example, consider the basis of two qubits $|0\rangle$ and $|1\rangle$ with the correspong sum

$$\sum_{i=0}^{1} \boldsymbol{P}_i = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}.$$

Based on the spectral decomposition discussed above, we can define the probability of eigenvalue λ_i as

$$\mathrm{Prob}(\lambda_i) = |\boldsymbol{P}_i|\psi\rangle|^2,$$

where $|\psi_{\boldsymbol{a}}\rangle$ is a quantum state representing the system prior to a specific measurement.

Total probability

We can rewrite this as

$$\mathrm{Prob}(\lambda_i) = \langle\psi|\boldsymbol{P}_i^\dagger \boldsymbol{P}_i|\psi\rangle = \langle\psi|\boldsymbol{P}_i|\psi\rangle.$$

The total probability for all measurements is the sum overt all probabilities

$$\sum_{i=0}^{n-1} \mathrm{Prob}(\lambda_i) = 1.$$

We can in turn define the post-measurement normalized pure quantum state as, for the specific outcome λ_i, as

$$|\psi'\rangle = \frac{\boldsymbol{P}_i|\psi\rangle}{\sqrt{\langle\psi|\boldsymbol{P}_i|\psi\rangle}}.$$

Binary example system

As an example, consider the binary system states $|0\rangle$ and $|1\rangle$ with corresponding projection operators

$$\boldsymbol{P}_0 = |0\rangle\langle 0|,$$

and

$$\boldsymbol{P}_1 = |1\rangle\langle 1|,$$

with the properties

$$\sum_{i=0}^{1} \boldsymbol{P}_i^\dagger \boldsymbol{P}_1 = \boldsymbol{I},$$

$$\boldsymbol{P}_0^\dagger \boldsymbol{P}_0 = \boldsymbol{P}_0^2 = \boldsymbol{P}_0,$$

and

$$\boldsymbol{P}_1^\dagger \boldsymbol{P}_1 = \boldsymbol{P}_1^2 = \boldsymbol{P}_1.$$

Superposition state

Assume thereafter that we have a state $|\psi\rangle$ which is a superposition of the above two qubit states

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle.$$

The probability of finding either $|0\rangle$ or $|1\rangle$ is then

$$\boldsymbol{P}_{\psi(0)} = \langle\psi|\boldsymbol{P}_0^\dagger \boldsymbol{P}_0|\psi\rangle = |\alpha|^2,$$

and similarly we have

$$\boldsymbol{P}_{\psi(1)} = \langle\psi|\boldsymbol{P}_1^\dagger \boldsymbol{P}_1|\psi\rangle = |\beta|^2.$$

More derivations

If we set

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

we have $|\alpha|^2 = |\beta|^2 = 1/2$. In general for this system we have

$$|\psi_0'\rangle = \frac{\boldsymbol{P}_0|\psi\rangle}{\sqrt{\langle\psi|\boldsymbol{P}_0|\psi\rangle}} = \frac{\alpha}{|\alpha|}|0\rangle,$$

and

$$|\psi_1'\rangle = \frac{\boldsymbol{P}_1|\psi\rangle}{\sqrt{\langle\psi|\boldsymbol{P}_1|\psi\rangle}} = \frac{\beta}{|\beta|}|1\rangle.$$

Final result

In general we have that

$$\boldsymbol{P}_{\psi(x)} = \langle\psi|\boldsymbol{P}_x^\dagger \boldsymbol{P}_x|\psi\rangle, ,$$

which we can rewrite as

$$\mathrm{Prob}(\psi(x)) = \mathrm{Tr}\left[\boldsymbol{P}_x^\dagger \boldsymbol{P}_x|\psi\rangle\langle\psi|\right].$$

Example

The last equation can be understood better through the following example with a state $|\psi\rangle$

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle,$$

which results in a projection operator

$$|\psi\rangle\langle\psi| = \begin{bmatrix} |\alpha|^2 & \alpha\beta^* \\ \alpha^*\beta & |\beta|^2 \end{bmatrix}.$$

Computing matrix products

We have that

$$\boldsymbol{P}_0^\dagger \boldsymbol{P}_0 = \boldsymbol{P}_0 = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix},$$

and computing the matrix product $\boldsymbol{P}_0|\psi\rangle\langle\psi|$ gives

$$\boldsymbol{P}_0|\psi\rangle\langle\psi| = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} |\alpha|^2 & \alpha\beta^* \\ \alpha^*\beta & |\beta|^2 \end{bmatrix} = \begin{bmatrix} |\alpha|^2 & \alpha\beta^* \\ 0 & 0 \end{bmatrix},$$

and taking the trace of this matrix, that is computing

$$\mathrm{Prob}(\psi(0)) = \mathrm{Tr}\left[\boldsymbol{P}_0^\dagger \boldsymbol{P}_0 |\psi\rangle\langle\psi|\right] = |\alpha|^2,$$

we obtain the same results as the one we had earlier by computing the probabliblity for 0 given by the expression

$$\boldsymbol{P}_{\psi(0)} = \langle\psi|\boldsymbol{P}_0^\dagger \boldsymbol{P}_0|\psi\rangle = |\alpha|^2.$$

Outcome probability

It is straight forward to show that

$$\text{Prob}(\psi(1)) = \text{Tr}\left[\boldsymbol{P}_1^\dagger \boldsymbol{P}_1 |\psi\rangle\langle\psi|\right] = |\beta|^2,$$

which we also could have obtained by computing

$$\boldsymbol{P}_{\psi(1)} = \langle\psi|\boldsymbol{P}_1^\dagger \boldsymbol{P}_1|\psi\rangle = |\beta|^2.$$

We can now extend these expressions to the complete ensemble of measurements. Using the spectral decomposition we have that the probability of an outcome $p(x)$ is

$$p(x) = \sum_{i=0}^{n-1} p_i \boldsymbol{P}_{\psi_i(x)},$$

where p_i are the probabilities of a specific outcome. Add later a digression on marginal probabilities.

With these prerequisites we are now ready to introduce the density matrices, or density operators.

Density matrices/operators

The last equation can be rewritten as

$$p(x) = \sum_{i=0}^{n-1} p_i \boldsymbol{P}_{\psi_i(x)} = \sum_{i=0}^{n-1} p_i \mathrm{Tr}\left[\boldsymbol{P}_x^\dagger \boldsymbol{P}_x |\psi_i\rangle\langle\psi_i|\right],$$

and we define the **density matrix/operator** as

$$\rho = \sum_{i=0}^{n-1} p_i |\psi_i\rangle\langle\psi_i|,$$

we can rewrite the first equation above as

$$p(x) = \mathrm{Tr}\left[\boldsymbol{P}_x^\dagger \boldsymbol{P}_x \rho\right].$$

If we can define the state of a system in terms of the density matrix, the probability of a specific outcome is then given by

$$p(x)_\rho = \mathrm{Tr}\left[\boldsymbol{P}_x^\dagger \boldsymbol{P}_x \rho\right].$$

Properties of density matrices

A density matrix in a Hilbert space with n states has the following properties (which we state without proof)

1. There exists a probability $p_i \geq 0$ with $\sum_i p_i = 1$,
2. There exists an orthonormal basis ψ_i such that we can define $\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$,
3. We have $0 \leq \rho^2 \leq 1$ and
4. The norm $||\rho||_2 \leq 1$.

With the density matrix we can also define the state the system collapses to after a measurement, namely

$$\rho'_x = \frac{\boldsymbol{P}_x \rho \boldsymbol{P}_x^\dagger}{\mathrm{Tr}[\boldsymbol{P}_x^\dagger \boldsymbol{P}_x \rho]}.$$

Representation of states and Hamiltonians

Before we proceed we need several other definitions. Throughout these lectures we will assume that the interacting part of the Hamiltonian can be approximated by a two-body interaction. This means that our Hamiltonian can be written as the sum of a onebody part, which includes kinetic energy and an eventual external field, and a twobody interaction

$$\hat{H} = \hat{H}_0 + \hat{H}_I = \sum_{i=1}^{N} \hat{h}_0(x_i) + \sum_{i<j}^{N} \hat{v}(r_{ij}), \tag{1}$$

with the onebody part

$$H_0 = \sum_{i=1}^{N} \hat{h}_0(x_i). \tag{2}$$

Typical onebody Hamiltonians

The onebody part $u_{\mathrm{ext}}(x_i)$ is normally approximated by a harmonic oscillator potential or the Coulomb interaction an electron feels from the nucleus. However, other potentials are fully possible, such as one derived from the self-consistent solution of the Hartree-Fock equations or density functional theories.

Symmetries

Our Hamiltonian is invariant under the permutation (interchange) of two particles. Since we deal with fermions however, the total wave function is antisymmetric. Let $\hat{P}$ be an operator which interchanges two particles. Due to the symmetries we have ascribed to our Hamiltonian, this operator commutes with the total Hamiltonian,

$$[\hat{H}, \hat{P}] = 0,$$

meaning that $\Psi_\lambda(x_1, x_2, \dots, x_N)$ is an eigenfunction of $\hat{P}$ as well, that is

$$\hat{P}_{ij}\Psi_\lambda(x_1, x_2, \dots, x_i, \dots, x_j, \dots, x_N) = \beta\Psi_\lambda(x_1, x_2, \dots, x_i, \dots, x_j, \dots, x_N),$$

where β is the eigenvalue of $\hat{P}$. We have introduced the suffix ij in order to indicate that we permute particles i and j. The variable N refers to the number of particles. The Pauli principle tells us that the total wave function for a system of fermions has to be antisymmetric, resulting in the eigenvalue $\beta = -1$. The variable N represents the number of particles.

Fermions

If we deal with fermions, we assume that we can approximate the exact eigenfunction with a Slater determinant

$$\Phi(x_1, x_2, \ldots, x_N, \alpha, \beta, \ldots, \sigma) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \psi_\alpha(x_1) & \psi_\alpha(x_2) & \ldots & \ldots & \psi_\alpha(x_N \\ \psi_\beta(x_1) & \psi_\beta(x_2) & \ldots & \ldots & \psi_\beta(x_N \\ \ldots & \ldots & \ldots & \ldots & \ldots \\ \ldots & \ldots & \ldots & \ldots & \ldots \\ \psi_\sigma(x_1) & \psi_\sigma(x_2) & \ldots & \ldots & \psi_\sigma(x_N \end{vmatrix} \tag{3}$$

where x_i stand for the coordinates and spin values of a particle i and $\alpha, \beta, \ldots, \gamma$ are quantum numbers needed to describe remaining quantum numbers. This ansatz for the computational basis is often based on single-particle functions which are eigenfunctions of a part of the total Hamiltonian. Most frequently, these single-particle basis functions are eigenpairs of the non-interacting part of the Hamiltonian (normally defined by kinetic and external potential operators).

Ansatz for states

For Fermions (identical and indistinguishable particles) we will form an ansatz for a given state in terms of so-called Slater determinants determined by a chosen basis of single-particle functions.
For a given $n \times n$ matrix A we can write its determinant

$$det(\mathrm{A}) = |\mathrm{A}| = \begin{vmatrix} a_{11} & a_{12} & \dots & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & \dots & a_{2n} \\ \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots \\ a_{n1} & a_{n2} & \dots & \dots & a_{nn} \end{vmatrix},$$

in a more compact form as

$$|\mathrm{A}| = \sum_{i=1}^{n!} (-1)^{p_i} \hat{P}_i a_{11} a_{22} \dots a_{nn},$$

where $\hat{P}_i$ is a permutation operator which permutes the column indices $1, 2, 3, \dots, n$ and the sum runs over all $n!$ permutations. The quantity p_i represents the number of transpositions of column indices that are needed in order to bring a given permutation back to its initial ordering, in our case given by $a_{11} a_{22} \dots a_{nn}$ here.

Simple fermionic example

A simple 2×2 determinant illustrates this. We have

$$det(\mathrm{A}) = \begin{vmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{vmatrix} = (-1)^0 a_{11} a_{22} + (-1)^1 a_{12} a_{21},$$

where in the last term we have interchanged the column indices 1 and 2. The natural ordering we have chosen is $a_{11} a_{22}$.

Using an ONB

We define our new single-particle basis (this is a normal approach for Hartree-Fock theory) by performing a unitary transformation on our previous basis (labelled with greek indices) as

$$|\psi\rangle_i = \sum_j u_{ij} |\phi\rangle_j.$$

If the basis has infinitely many solutions, we need to truncate the above sum. We assume that the basis $|\phi\rangle_j$ is orthogonal.
If we stay with determinants, a feature which will become useful is to expand a new determinant in terms of a previous one that is defined by a given set of single-particle state functions. As discussed above, we can define a new basis that is a linear combination of another basis (assumed to be orthogonal and normalized). This means that if the coefficients u_{ij} belong to a unitary or orthogonal orthogonality is preserved, as discussed above. This propertry is extremely useful when we build up a basis of many-body Stater determinant based states.

Simple Hamiltonian models

In order to study get started with coding, we will study two simple Hamiltonian systems, one which we can use for a single qubit systems and one which has as basis functions a two-qubit system. These two simple Hamiltonians exhibit also something which is called level crossing, a feature which we will use in later studies of entanglement.
We study first a simple two-level system. Thereafter we extend our model to a four-level system which can be interpreted as composed of two separate (not necesseraly identical) subsystems.
We let our hamiltonian depend linearly on a strength parameter z

$$H = H_0 + \lambda H_{\mathrm{I}},$$

with $\lambda \in [0, 1]$, where the limits $\lambda = 0$ and $\lambda = 1$ represent the non-interacting (or unperturbed) and fully interacting system, respectively.

Defining a computational basis

The model is an eigenvalue problem with only two available states, which we label $|0\rangle$ and $|1\rangle$, respectively. Below we will let state $|0\rangle$ represent the lowest state (often referred to as model-space state) with its pertinent eigenvalue and eigenvector whereas state $|1\rangle$ represents the eigenvalue of the excluded space. The non-interacting solutions to our problem are

$$H_0|0\rangle = \epsilon_0|0\rangle, \tag{4}$$

and

$$H_0|1\rangle = \epsilon_1|1\rangle, \tag{5}$$

with $\epsilon_0 < \epsilon_1$. We label the off-diagonal matrix elements X, while $X_0 = \langle 0|H_I|0\rangle$ and $X_1 = \langle 1|H_1|1\rangle$.

Analytical solutions

The solution to the eigenvalue problem
labeleq:twolevelH

$$\begin{pmatrix} \epsilon_0 + \lambda X_0 & \lambda X \\ \lambda X & \epsilon_1 + \lambda X_1 \end{pmatrix} \tag{6}$$

yields

$$\begin{aligned} E(\lambda) = \quad & \tfrac{1}{2}\left\{\epsilon_0 + \epsilon_1 + \lambda X_0 + \lambda X_1 \pm (\epsilon_1 - \epsilon_0 + \lambda X_1 - \lambda X_0)\right. \\ & \left. \times \sqrt{1 + \frac{4\lambda^2 X^2}{(\epsilon_1 - \epsilon_0 + \lambda X_1 - \lambda X_0)^2}} \right\}. \end{aligned} \tag{7}$$

Numerical examples

For this part we recommend using the jupyter-notebook.

In the results below we set the parameters $\epsilon_0 = 0$, $\epsilon_1 = 4$, $X_0 = -X_1 = 3$ and $X = 0.2$. This eigenvalue problem can easily be rewritten in terms of the standard Pauli matrices. The non-interacting solutions represent our computational basis. Pertinent to our choice of parameters, is that at $\lambda \geq 2/3$, the lowest eigenstate is dominated by $|1\rangle$ while the upper is $|0\rangle$. At $\lambda = 1$ the $|0\rangle$ mixing of the lowest eigenvalue is 1% while for $\lambda \leq 2/3$ 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 X represents the strength of the coupling between the model space and the excluded space. The following code computes and plots the eigenvalues.

```
%matplotlib inline

from  matplotlib import pyplot as plt
import numpy as np
dim = 2
#Setting up a tridiagonal matrix and finding eigenvectors and eigenval
Hamiltonian = np.zeros((dim,dim))
#number of lambda values
```

First exercise set

The exercises we present each week are meant to build the basis for the two projects we will work on during the semester. The first project deals with implementing the so-called **Variational Quantum Eigensolver** algorithm for finding the eigenvalues and eigenvectors of selected Hamiltonians. Feel free to use the above codes in order to get started.

Write a function which sets up a one-qubit basis and apply the various Pauli matrices to these basis states.

Apply the Hadamard and Phase gates to the same one-qubit basis states and study their actions on these states.

We define a symmetric matrix $H \in \mathbb{R}^{2\times 2}$

$$H = \begin{bmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{bmatrix},$$

We let $H = H_0 + H_I$, where

$$H_0 = \begin{bmatrix} E_1 & 0 \\ 0 & E_2 \end{bmatrix},$$

is a diagonal matrix. Similarly,

$$H_I = \begin{bmatrix} V_{11} & V_{12} \\ V_{21} & V_{22} \end{bmatrix},$$

where V_{ij} represent various interaction matrix elements. We can view H_0 as the non-interacting solution

$$H_0|0\rangle = E_1|0\rangle, \tag{8}$$

and

$$H_0|1\rangle = E_2|1\rangle, \tag{9}$$

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

a) Show that you can rewrite the above Hamiltonian in terms of

Using the one-qubit basis write a code which sets up a two-qubit basis and encodes this basis.

Use the Hamiltonian for the two-qubit example to find the eigenpairs as functions of the interaction strength λ and study the final eigenvectors as functions of the admixture of the original basis states.

The next lecture, January 31

In our next lecture, we will discuss

1. Reminder and review of density matrices and measurements
2. Schmidt decomposition and entanglement
3. Discussion of entropies, classical information entropy (Shannon entropy) and von Neumann entropy

Chapters 3 and 4 of Scherer's text contains useful discussions of several of these topics.