Dynamics at an exceptional point in an interacting quantum dot system

William Samuelson

August 9, 2022

1 Introduction

2 Theory

The theory part of the thesis is divided into five major sections. Firstly, a brief overview of the theory behind transport through quantum dots is given. Then the focus is put on some of the tools used in open quantum systems, ultimately ending in a section about quantum master equations. The final three sections will explain the notion of exceptional points, the Jordan normal form and lastly presenting a useful analytic form of the solution of a system of ordinary differential equations.

2.1 Transport through quantum dots

2.1.1 Single electron transistor

To begin understanding the transport of electrons through a system of quantum dots, it is insightful to first study a simple system, known as a single electron transistor. Consider a single quantum dot with N electrons capacitively coupled to a gate and coupled to source and drain reservoirs through tunnel junctions. (FIGURE) The main transport properties of the system can then be understood in terms of the chemical potentials of the quantum dot and the source and drain reservoirs. These are often depicted in electro-chemical potential diagrams, see figure X. There, $\mu(N)$ is the energy required to add the Nth electron to the quantum dot, and μ_S and μ_D are the Fermi levels of the source and drain. The shaded areas represent the Fermi-Dirac distributions of the source and drain.

Using this picture, the electron transport through the quantum dot can be easily visualized. If the chemical potential levels are located as in figure Y, $\mu(N+1)$ is below μ_S, and an electron will likely tunnel from the source onto the dot, increasing the number of electrons on the dot from N to $N+1$. After the tunneling event, there is an even lower chemical potential available for the electron, μ_D, and the electron will with a high probability leave the quantum dot and enter the drain. In this fashion, the system will cycle through having N and $N+1$ electrons on the dot, producing a current.

It turns out that $\mu(N)$ depends linearly on the gate voltage V_G, so by changing it, the "ladder" of states in figure X can be lowered or raised. The drain voltage V_D on the other hand, changes the spacing between μ_S and μ_D. Through these two processes, it is possible to change the electro-chemical potential landscape and therefore control the current through the system.

2.1.2 Master equations

An important tool for simulating the current through a quantum dot system is the master equation approach. A classical master equation is defined by

$$\frac{\mathrm{d}p_i}{\mathrm{d}t} = \text{Rate of entering state } i - \text{Rate of leaving state } i = \sum_j R_{ji} p_j - \sum_j R_{ij} p_i \tag{1}$$

with probabilities p_i of being in state i, and transition rates R_{ij} describing the rate of transitions from state i to state j. For the single electron transistor, the states i correspond to the number of electrons on the dot. The transition rates are typically related to the Fermi-Dirac distributions of the reservoirs and the tunneling rates of the barriers.

Collecting the rate equations for each i and adding the condition $\sum_i p_i = 1$, a system of ordinary differential equations is obtained. This can be solved numerically using standard methods, such as the Runge-Kutta method. Once the probabilities are obtained, the evolution of the current can be calculated by considering the amount of charge tunneling through the barriers at each time point.

While a classical master equation may give accurate results for a quantum system, it leaves out some important details. A *quantum master equation* generalizes the notion of a classical master equation in the following sense: The unknown in a quantum master equation does not only contain the probabilities p_i of being in a quantum state $|\psi_i\rangle$, but also *coherences*, which are necessary to describe a quantum system fully. This topic will further be delved upon in section 2.2.3.

2.2 The theory of open quantum systems

Open quantum systems are systems which are non-isolated and connected to some sort of environment. Often, it considers a total system consisting of the (sub)system of interest, and an environment. The total system is closed, and therefore it obeys the regular quantum mechanical equations of motion. The goal of the theory of open quantum systems is to infer the equation of motion of the smaller system from the equations of the total system.

2.2.1 The von Neumann equation and the reduced density operator

An important tool used in open quantum theory is the *density operator* $\hat{\rho}$. In open quantum systems, it might only be known that the system is in states $|\psi_i\rangle$ with probabilities p_i. Then the system is said to be in an *ensemble* $\{|\psi_i\rangle, p_i\}$. The density operator describes this information in a compact way:

$$\hat{\rho} = \sum_i p_i |\psi_i\rangle \langle\psi_i| . \tag{2}$$

Fixing a basis $\{|\phi_i\rangle\}$, the density operator can be represented by a matrix with elements $\rho_{ij} = \langle\phi_i|\hat{\rho}|\phi_j\rangle$. The diagonal elements ρ_{ii} represents classical probabilities of being in a state $|\phi_i\rangle$ and the off-diagonal elements ρ_{ij} are the coherences of the system.

The average measured value of an observable $\hat{O}$ of an ensemble represented by $\hat{\rho}$ can be shown to be

$$\langle \hat{O} \rangle = \mathrm{Tr}(\hat{\rho}\hat{O}). \tag{3}$$

From the density operator one can therefore extract all signifiant information from the ensemble. It is also possible to calculate how the density operator evolves over time. Under a Hamiltonian $\hat{H}$, the evolution is given by the von Neumann equation

$$i\hbar \frac{\mathrm{d}\hat{\rho}}{\mathrm{d}t} = [\hat{H}, \hat{\rho}] \equiv \mathcal{L}\hat{\rho}, \tag{4}$$

where $\mathcal{L}$ is the *Liouvillian superoperator*, or just the Liouvillian.

Connecting back to the mentioned goal of open quantum theory - How does one calculate the evolution of the density operator describing a subsystem connected to an environment? This question is solved by the *reduced density operator*. If the total system T consists of a subsystem S and an environment E, then the reduced density matrix for the subsystem is given by

$$\hat{\rho}_S = \mathrm{Tr}_E(\hat{\rho}_T), \tag{5}$$

where Tr_E is the partial trace over the environment. It is therefore possible to "trace out" the environment and obtain a density operator for the subsystem of interest which contain all measurement statistics of interest. This process is at the core of open quantum theory.

2.2.2 The Fock-Liouville space

The Liouvillian $\mathcal{L}$ in equation 4 is an operator acting on an operator, which is why it is called a superoperator. To be able to more easily handle the Liouvillian, it is possible to treat it as a normal operator represented by a matrix, acting on a Hilbert space spanned by the density matrices. The density matrix is therefore effectively transformed into a vector, usually written as $|\rho\rangle\rangle$, with a scalar product $\langle\langle \rho_1 | \rho_2 \rangle\rangle$. The Hilbert space spanned by these vectors is called the Fock-Liouville space.

2.2.3 The Lindblad Master equation

2.3 Exceptional points

In quantum mechanics, a common way to perform calculations is to diagonalize the matrix representation of the Hamiltonian. The diagonalization process can be understood a change of basis to linearly independent eigenvectors. In this basis, the linear transformation of the matrix is very simple: it scales each eigenvector by the corresponding eigenvalue. The matrix in the new basis is therefore diagonal, explaining the name of the process. For a matrix A and its diagonal form D, this can be written as

$$A = SDS^{-1}, \tag{6}$$

where $S = (v_1, \dots v_n)$ consists of the eigenvectors. The diagonalization process can always be done for Hamiltonians in quantum mechanics. The reason is that the Hamiltonian is an observable, which by the postulates in quantum mechanics always are Hermitian. This in turn means that the matrix representation is normal, and therefore diagonalizable.

In Liouvillian physics, there are non-Hermitian parts in the Liouvillian superoperator. The matrix representation of the Liouvillian is hence not necessarily diagonalizable, but can be defective. If a matrix is defective, two or more eigenvalues and their corresponding eigenvectors coalesce.

The Liouvillian matrix often depends on a set of parameters describing the system. If a point in this parameter space produces a defective matrix, the point is called an *exceptional point* (EP). Exceptional points can be of different *orders*, reflecting how many eigenvectors coalesce at the point. For example, if three eigenvectors coalesce, the EP is said to be of order three.

2.4 Jordan normal form

For a defective matrix, there does not exist a basis of eigenvectors, and the diagonalization process is not possible. Fortunately, there is a notion of an "almost diagonal" form, called the Jordan normal form. Recall that in the diagonalizable case, the basis was changed to the linearly independent eigenvectors. To construct the Jordan form for a defective matrix, this basis has to be completed in some way to span the full space. This can be done using *Jordan chains*, which for each defective eigenvector r_i with eigenvalue λ_i, consists of vectors r_i', r_i'' ... defined by equation 7. The length of chain, n_i, is the same as the order of the corresponding EP.

$$\begin{aligned} (A - \lambda_i I) r_i &= 0 \\ (A - \lambda_i I) r_i' &= r_i \\ (A - \lambda_i I) r_i'' &= r_i' \\ &\vdots \quad . \end{aligned} \tag{7}$$

Using this new basis and creating the change-of-basis matrix M by forming

$$M = (\boldsymbol{r}_1 \dots \boldsymbol{r}_q), \quad \text{where } \boldsymbol{r}_i = (r_i,\ r_i',\ r_i'' \dots), \tag{8}$$

the Jordan normal form J of the matrix A is obtained:

$$A = MJM^{-1},$$

$$\text{where } J = \begin{bmatrix} J_{n_1}(\lambda_1) & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & J_{n_q}(\lambda_q) \end{bmatrix} \quad \text{and } J_{n_i}(\lambda_i) = \begin{bmatrix} \lambda_i & 1 & \dots & 0 \\ \vdots & \ddots & \ddots & \vdots \\ \vdots & & \ddots & 1 \\ 0 & \dots & \dots & \lambda_i \end{bmatrix}. \tag{9}$$

The Jordan form hence consist of q blocks on the diagonal, each block of size n_i consisting of its eigenvalue on the diagonal and ones on the super diagonal. Note that if all blocks are of size one, i.e there are no exceptional points, the Jordan form is diagonal.

2.5 Solution of ODEs

An ordinary differential equation (ODE) is a linear differential equation of the form $x' = Ax$. Often, the unknown x is a vector, and A a matrix. The solution can be written as a matrix exponential in the following way:

$$x(t) = e^{At}x(0), \text{ where } e^{At} = \sum_{k=0}^{\infty} \frac{(At)^k}{k!}. \tag{10}$$

The matrix exponential can be simplified using Jordan decomposition. It can be shown that $e^{At} = Me^{Jt}M^{-1}$ where

$$\begin{aligned} e^{Jt} &= \begin{bmatrix} e^{J_{n_1}(\lambda_1)t} & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & e^{J_{n_q}(\lambda_q)t} \end{bmatrix}, \text{ and} \\ e^{J_{n_i}(\lambda_i)t} &= e^{\lambda_i t} \begin{bmatrix} 1 & t & \dots & t^{n_i-1}/(n_i-1)! \\ \vdots & \ddots & \ddots & \vdots \\ \vdots & & \ddots & t \\ 0 & \dots & \dots & 1 \end{bmatrix}. \end{aligned} \tag{11}$$

In general, the matrix exponential therefore consists of entries with terms of the form $t^k e^{\lambda_i t}$. Note that if A is diagonalizable, all blocks are of size one and the entries consist of pure exponentials on the diagonal.

Using this result, the solution can be written as

$$x(t) = Me^{Jt}M^{-1}x(0). \tag{12}$$

This can further be decomposed if one considers the generalized modes of the system. Suppose first that the initial state is in a linear combination of vectors in one of the Jordan chains, $x(0) = a_1 r_i + a_2 r_i' + a_3 r_i'' + \dots = \boldsymbol{r}_i a$, where $a = (a_1, \dots a_{n_i})^T$ is a constant vector and $\boldsymbol{r}_i$ is defined in equation 8. By rewriting M^{-1} as (EXPLAIN IN PREV SECTION?)

$$M^{-1} = \begin{bmatrix} \boldsymbol{l}_1 \\ \vdots \\ \boldsymbol{l}_{n_i} \end{bmatrix} \tag{13}$$

and using equation 12, the solution can be written as (MAYBE WRITE MORE STEPS)

$$x(t) = Me^{Jt}M^{-1}x(0) = Me^{Jt}\begin{bmatrix} \boldsymbol{l}_1 \\ \vdots \\ \boldsymbol{l}_{n_i} \end{bmatrix} \boldsymbol{r}_i a = \boldsymbol{r}_i e^{J_{n_i}(\lambda_i)t} a, \tag{14}$$

since $\boldsymbol{l}_j \boldsymbol{r}_i = \delta_{ij} I$, where I is the $n_j \times n_i$ identity matrix. Hence, the solution stays in the space spanned by the initial condition throughout the evolution. For an arbitrary initial condition, the solution can be written as a sum over the generalized modes:

$$x(t) = \sum_{i=1}^{q} \boldsymbol{r}_i e^{J_{n_i}(\lambda_i)t} \boldsymbol{l}_i x(0). \tag{15}$$