The density matrix and its application to quantum transport

PART I : BASIC CONCEPTS AND METHODS

PART II : QUANTUM TRANSPORT

CH. 4: DIAGRAMMATIC APPROACES

Literature:

- K. Blum: Density matrix theory and its applications 2nd Ed. Plenum Press (1996)

- H.-P. Breuer and F. Petruccione: The theory of open quantum systems, Oxford University Press (2002)

- H. Bruus and K. Flensberg: Many-body quantum theory in condensed matter. Oxford graduate texts (2007)

- C. Beenakker: Theory of Coulomb-blockade oscillations in the conductance of a quantum dot, Phys. Rev. B 44, 1646 (1991)

- C. Timm: Tunnelling through molecules and quantum dots: master equation approaches, Phys. Rev. B, 195417 (2008)

- S. Koller et al.: Density operator approaches to transport through interacting quantum dots: simplification in fourth-order perturbation theory, Phys. Rev. B 82, 045316 (2010)

- H. Schoeller: Transport theory of interacting quantum dots, Habilitationsschrift (1997)

- S. Koller: Spin phenomena and higher order effects in transport across interacting quantum dots. PhD thesis Regensburg (2009)

- D. Mantelli: Analytical and numerical study of quantum impurity systems in the intermediate and strong coupling regimes PhD thesis Regensburg (2016)

<u>Exercises</u>: The exercise sheet is posted on-line each Friday on my homepage (Teaching → Density Matrix Theory ST 2018) and will be discussed in class on the following Friday.
The evaluation of the exercises will be through the crossing and random choice method. Regular participation to the class and at least 50% of the exercises are the requirements to pass the course (obtain the credit points)

Fixed class and exercise rooms and times:

Classes:	Tuesdays	$12 \overset{\text{s.t.}}{-} 14$	5.0.20
	Thursdays	$10 \overset{\text{c.t}}{-} 12$	9.1.09
Exercises	Fridays	$10 \overset{\text{c.t}}{-} 12$	5.0.21

PART I

BASIC CONCEPTS AND METHODS

Chapter 1: GENERAL DENSITY MATRIX THEORY

1.1. Pure and mixed states

In classical mechanics a microscopic definition of a states involves the knowledge of the position and momentum of all particles comprising the system

▲ Which is the "maximum available information" obtained by measuring a quantum mechanical system?

In QM a precise simultaneous measurement of two physical variables is only possible if the variables are NOT conjugated (i.e. the associated operators commute). In other words, if $[\hat{Q}_1, \hat{Q}_2] = 0$ => it is possible to find states $|\psi\rangle$ such that $\hat{Q}_1|\psi\rangle = q_1|\psi\rangle$ and $\hat{Q}_2|\psi\rangle = q_2|\psi\rangle$. $|\psi\rangle$ is both an eigenstate of $\hat{Q}_1$ and $\hat{Q}_2$.

=> In general the maximum available information that can be achieved consists of the eigenvalues $q_1, \dots, q_N$ of the largest set of mutually commuting independent observables $Q_1, \dots, Q_N$. The system is completely specified by assigning the state vector:

$$|\psi\rangle = |q_1, q_2, \dots, q_N\rangle$$ to it.

Def: A PURE STATE is a state of maximum knowledge

U. Fano 1957

Note: The choice of a complete set of commuting operators is not unique.

Thus, $|\psi\rangle$ can be specified by the eigenvalues $q_1, q_2, \dots, q_N$ of a complete operator set or by giving the amplitudes a_n ($\in \mathbb{C}$) and the orthonormal eigenstates basis $|\phi_n\rangle$ of another set of observables

$$|\psi\rangle = \sum_n a_n |\phi_n\rangle \quad (1.1)$$

$\{|\phi_n\rangle\}$ is constructed as $|\{\phi_1, \dots, \phi_N\}\rangle$ with all possible eigenvalues of a complete set of observables.

Refresh: $\{|\phi_n\rangle\}$ orthonormal basis implies $\langle\phi_n|\phi_m\rangle = \delta_{nm}$ and

$$1 = \sum_n |\phi_n\rangle\langle\phi_n|$$

The normalization of $|\psi\rangle$ implies $1 = \langle\psi|\psi\rangle = \sum_n |a_n|^2 \quad (1.2)$

$\Rightarrow$ $|a_n|^2$ is the probability that a measurement will give the result $(\phi_1, \dots, \phi_N)$, or, in other terms the probability to find the system in $|\phi_n\rangle$.

▲ $\exists$s it feasible to completely prepare a system in a pure state?

Similarly to classical mechanics, in most cases we only have a partial knowledge of the quantum mechanical state of a system.

$\Rightarrow$ The state of the system is not pure (at least we cannot tell since, practically, we cannot prepare it). But we can say that the system has certain <u>probabilities</u> $w_1, \dots, w_M$ of being in the pure states $|\psi_1\rangle, \dots |\psi_M\rangle$, respectively.

<u>Def</u>: Systems that cannot be characterized by a single state vector are called <u>statistical mixtures</u>

▲ Is there a consequence of this distinction between pure and mixed states in the measurement of a generic observable Q?

- pure state: $|\psi\rangle$

  $|\psi\rangle$ is an eigenstate of the observable Q
  $\Downarrow$
  each measurement give the same eigenvalue q.

  $|\psi\rangle$ is not an eigenstate of the observable Q
  $\Downarrow$
  the measurements give different results. The average is given by the expectation value $\langle\hat{Q}\rangle_{pure} = \langle\psi|\hat{Q}|\psi\rangle$ (1.3)

- statistical mixture: The measurements give different results whose average is given by the expectation value

$$\langle\hat{Q}\rangle_{mix} = \sum_n W_n \langle\psi_n|\hat{Q}|\psi_n\rangle \quad (1.4)$$

For a pure state the (possible) scattering of the measurement results has only a QM explanation as uncontrollable perturbation introduced by the very same measurement. For a statistical mixture one adds to this effect the lack of knowledge over the system.