The density matrix and its application to the quantum transport (52442)

First meeting:

Wednesday, 16th October, 11:15

PHY 4.1.13

The course is an introduction to the theory of open systems in the reduced density matrix description. Basic concepts of quantum transport are also presented. Fundamental transport properties of interacting nano-junctions are analyzed using the Liouville approach. The theory is applicable to a large variety of systems and several examples will be considered.

Lectures:	*Wed*	*11:00 c.t.*, PHY 2.0.31
	Thu	*10:00 s.t.*, PHY 2.1.29
Exercises:	*Fri*	*14:00 c.t.*, PHY 9.1.10

Institute of Theoretical Physics, University of Regensburg

The density matrix and its application to quantum transport

PART I : BASIC CONCEPTS AND METHODS

CH. 1 : GENERAL DENSITY MATRIX THEORY

1.1 Pure and mixed states

1.2 The density matrix and its basic properties

1.3 Coherence vs. incoherence

1.4 Time evolution: Liouville-von Neumann equation

1.5 Systems in thermal equilibrium

CH. 2 : COUPLED SYSTEMS: THE REDUCED DENSITY MATRIX

2.1 Separability vs. non-separability

2.2 Emergence of irreversibility: the reduced density matrix (RDM)

2.3 Generalized master equation (GME) for the RDM
(System-bath model, Bath correlation functions and prop. kernels, Markov approx., Wangsness-Bloch-Redfield equations, Rotating wave approx., Pauli-master equation, Non-perturbative methods (Influence functional path integral.

2.4 The projector operator technique (Nakajima-Zwanzig equation)

2.5 The T-matrix approach

CH. 4: DIAGRAMMATIC APPROACHES

4.1: Iterative method and the Hilbert space description

4.2: Diagrammatic analysis in the time and energy domain

4.3: Fourth order GME: physical interpretation

4.4: Simple time diagrammatics in Liouville space

4.5 All orders resummations: dressed second order (DSO) and resonant time approximation (RTA)

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, PRB 82, 045316 (2010)

- 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)

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

<u>Exercises:</u> The exercise sheet is posted on-line each Thursday on my homepage (Teaching → Density Matrix Theory WT 19/20) and will be discussed in class of Friday of the following week.

The evaluation of the exercises will be through the crossing and random choice method. Regular participation to the class and at least 75% of the exercises are the requirements to obtain the credit points. Oral exam is offer for a grading.

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 state involves the knowledge of the position and momentum of all particles composing 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:

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

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.

* better: one of the largest sets

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 complete set of observables

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

$\{|\phi_n\rangle\}$ 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 $\quad 1 = \langle\psi|\psi\rangle = \sum_n |a_n|^2 \quad (1.2)$

$\Rightarrow$ $|a_n|^2$ 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 $|\phi_n\rangle$.

▲ Is 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.

Def: 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.

1.2. The density matrix and its basic properties

▲ Is there a formalism able to treat on an equal footing both pure states and statistical mixtures?

Def. The density operator describing a statistical mixture of states is defined as:

$$\hat{\rho} \equiv \sum_n W_n |\psi_n\rangle\langle\psi_n| \quad (1.5) \qquad \sum_n W_n = 1$$

Note: if the system is in a pure state $|\psi\rangle$ $\quad \hat{\rho} = |\psi\rangle\langle\psi|$ (1.5b) which is just a special case of (1.5).

Matrix representation Let us consider the ON basis set $\{|\phi_1\rangle, \dots, |\phi_N\rangle\}$ such that

$$|\psi_n\rangle = \sum_m a_m^{(n)} |\phi_m\rangle \quad \Rightarrow \quad \langle\psi_n| = \sum_m a_m^{(n)*} \langle\phi_m|$$

$$\Rightarrow \quad \hat{\rho} = \sum_n \sum_{m,m'} W_n a_m^{(n)} a_{m'}^{(n)*} |\phi_m\rangle\langle\phi_{m'}| \quad (1.6)$$

It follows as a def. of the density matrix

$$\rho_{ij} = \langle\phi_i|\hat{\rho}|\phi_j\rangle = \sum_n W_n a_i^{(n)} a_j^{(n)*} \qquad (1.7)$$

Properties of ρ:

i) $\rho_{ij} = \langle\phi_i|\hat{\rho}|\phi_j\rangle = \langle\phi_j|\hat{\rho}|\phi_i\rangle^* = \rho_{ji}^* \quad \Rightarrow \quad \rho$ is Hermitian

ii) The probability of finding the system in the pure state $|\psi\rangle$ after (complete) measurement is

$$W(\psi) = \underset{2}{\langle\psi|\hat{\rho}|\psi\rangle} = \underset{1}{\sum_n W_n |\langle\psi_n|\psi\rangle|^2} = \underset{3}{\sum_i \rho_{ii} |\langle\phi_i|\psi\rangle|^2}$$

iii] $\mathrm{Tr}\,\rho = \sum_i \rho_{ii} = 1$

proof: $\sum_i \rho_{ii} = \sum_i \sum_n W_n |a_i^{(n)}|^2 = \sum_n W_n \overbrace{\langle \psi_n | \underbrace{\left(\sum_i |\phi_i\rangle\langle\phi_i|\right)}_{=\mathbb{1}} | \psi_n \rangle}^{=1} = 1$

where the lower result stems from completness of $|\phi_i\rangle$, the upper from normalization of $|\psi_n\rangle$ and the last equality from W_n being a probability distribution. Note: the notation extends often to $\mathrm{Tr}\hat{\rho} \equiv \sum_n \langle \phi_n | \hat{\rho} | \phi_n \rangle = 1$

iv) The expectation value of any operator $\hat{Q}$ is:

$$\boxed{\langle \hat{Q} \rangle = \mathrm{Tr}\{\hat{\rho}\hat{Q}\} \quad (1.10)}$$

proof: $\langle \hat{Q} \rangle \overset{(1.4)}{=} \sum_n W_n \langle \psi_n | \hat{Q} | \psi_n \rangle = \sum_n \sum_{mm'} W_n a_m^{(n)} a_{m'}^{(n)*} \langle \phi_{m'} | \hat{Q} | \phi_m \rangle$

$$\overset{(1.7)}{=} \sum_{mm'} \rho_{mm'} \langle \phi_{m'} | \hat{Q} | \phi_m \rangle \overset{1.6}{=} \sum_{mm'} \langle m | \hat{\rho} | m' \rangle \langle m' | \hat{Q} | m \rangle$$

$$= \mathrm{Tr}\{\hat{\rho}\hat{Q}\}.$$

Note: More generally one can drop the normalization of $\{|\psi_n\rangle\}$ and define

$$\langle \hat{Q} \rangle = \frac{\mathrm{Tr}\{\hat{\rho}\hat{Q}\}}{\mathrm{Tr}\,\hat{\rho}} . \quad (1.10b)$$

In QM all information on the behavior of a system is given by the expectation values of a suitable set of operators. Since $\hat{\rho}$ allows to calculate such expectation values => $\hat{\rho}$ contains ALL physically relevant information on the system.

Note: Eq. (1.10) can be considered as an alternative definition of $\hat{\rho}$ compared to Eq. (1.7).

v) Iff a system is in a pure state $\text{Tr}\,\hat{\rho}^2 = (\text{Tr}\,\hat{\rho})^2$ (1.11)

proof: $\hat{\rho} = |\psi\rangle\langle\psi| \implies \hat{\rho}^2 = |\psi\rangle\underbrace{\langle\psi|\psi\rangle}_{=1}\langle\psi| = |\psi\rangle\langle\psi| = \hat{\rho}$

$\implies \text{Tr}\,\hat{\rho}^2 = \text{Tr}\,\hat{\rho}$. But $\text{Tr}\,\hat{\rho} = (\text{Tr}\,\hat{\rho})^2 = 1$

The opposite direction is slightly more difficult.

- in general $\text{Tr}\,\hat{\rho}^2 \leq (\text{Tr}\,\hat{\rho})^2$

proof: $\hat{\rho} = \sum_n W_n |\psi_n\rangle\langle\psi_n|$. Let us first assume a simpler form $\hat{\rho} = \sum_n W_n |\phi_n\rangle\langle\phi_n|$ (Diagonal in the orthonormal basis $\{|\phi_n\rangle\}$

$$\implies \hat{\rho}^2 = \sum_{n_1 n_2} W_{n_1} W_{n_2} |\phi_{n_1}\rangle\underbrace{\langle\phi_{n_1}|\phi_{n_2}\rangle}_{\delta_{n_1 n_2}}\langle\phi_{n_2}| = \sum_n W_n^2 |\phi_n\rangle\langle\phi_n|$$

$$\sum_n (W_n^2) \leq \underbrace{\left(\sum_n W_n\right)^2}_{= \sum_n W_n^2 + A(\{W_n\})}$$ simply because $W_n \geq 0 \ \forall n$.

$A \geq 0$

- $\text{Tr}\,\hat{\rho}^2 = \text{Tr}\,\hat{\rho}$?

$A(\{W_n\}) = \sum_n \sum_{m\neq n} W_n W_m$. $A = 0$ only if each term of the sum vanishes. Since $W_n = 0 \ \forall n$ is not allowed ($\text{Tr}\,\hat{\rho} = 1$!), the only possibility is that $\exists \bar{n} : W_{\bar{n}} = 1$ and $W_n = 0$ if $n \neq \bar{n}$.

$$\sum_n (W_n^2) = \left(\sum_n W_n\right)^2 \implies \hat{\rho} = |\phi_{\bar{n}}\rangle\langle\phi_{\bar{n}}| \implies \hat{\rho} \text{ represents a pure state.}$$

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