The density matrix and its application to quantum transport

PART I : BASIC CONCEPTS AND METHODS

PART II: QUANTUM TRANSPORT

CH. 4: ITERATIVE DIAGRAMMATIC APPROACH TO TUNNELING STRUCTURES

4.1 Generalized master equation (GME) for the RDM

4.2 The second order GME

4.3 The single electron tunneling (SET) regime

4.4 The fourth order GME

4.5 Differential conductance in fourth order

4.6 The resonant tunneling approximation

4.7 The Kondo regime

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 Univ. Press (2002)
- Yu. Nazarov and Ya. Blanter, Quantum Transport, Cambridge Univ. Press (2009)
- 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: Tunneling through molecules and quantum dots: master equation approaches. Phys. Rev. B 77, 195417 (2008)

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

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

Other recent research articles will be suggested upon request for further reading.

Exercises: The exercise sheet is given each Friday during the lecture and written solutions should be handed in by 12:00 of the Friday in the following week. The solution are discussed in the Exercises class of the following Tuesday.

Regular participation to the class + 50% of the exercises (more than half of the exercises in more than half of the sheets) is the requirement to pass the course.

Fixed class and exercise times:

Classes:	Mo	8:15 - 9:45	4.1.13	(Seminar room Richter)
	Fr	12:15 - 13:45	5.0.20	
Exercises:	Tu	10:15 - 11:45	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 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 $[\hat{Q}_1, \hat{Q}_2] = 0 \Rightarrow$ 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 $\hat{Q}_2$.

$\Rightarrow$ 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:

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

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.

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

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

<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.

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:

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

Note: if the system is in a pure state $|\psi\rangle$ $\hat{\rho} = |\psi\rangle\langle\psi|$ (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

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

Properties of ρ:

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

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

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

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

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

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 $\mathrm{Tr}\,\hat{\rho} \equiv \sum_n \langle \phi_n | \hat{\rho} | \phi_n \rangle$

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 $\{|\phi_n\rangle\}$ and define

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

In QM all information on the behaviour 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).

Illuminating example (1)

- Consider a system described by 2 quantum states: example an electron of which we neglect position or velocity.

- The number of real parameters necessary to describe the associated density matrix is 3. (In general N^2-1 where N is the size of the Hilbert space).

ρ_{ij} are N^2 but complex so, naively $2N^2$

ρ_{ii} are real and $\left(\sum_i \rho_{ii} = 1\right) \rightarrow -1$ since the diagonal entries satisfy Trρ = 1

$\rho_{ij} = \rho_{ji}^*$

N^2 since for the diagonal entries one needs only 1 number and 2 numbers for half of the off-diagonal entries.

- The density matrix can be defined by the expectation values of a given set of observables. For a spin system, the 3 components of the spin. $\hat{S}_i = \frac{\hbar}{2}\hat{\sigma}_i$ $\quad \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ $\quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$ $\quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

$$\langle \hat{S}_x \rangle = \frac{\hbar}{2}(\rho_{12}+\rho_{21}) = \hbar \,\mathrm{Re}\, \rho_{21}$$

$$\langle \hat{S}_y \rangle = \frac{\hbar}{2} i (\rho_{12}-\rho_{21}) = \hbar \,\mathrm{Im}\, \rho_{21}$$

$$\langle \hat{S}_z \rangle = \hbar \frac{\rho_{11}-\rho_{22}}{2}$$

$$1 = \rho_{11} + \rho_{22}$$

$$\Rightarrow \rho = \begin{pmatrix} \frac{1}{2} + \frac{\langle S_z \rangle}{\hbar} & \frac{1}{\hbar}(\langle S_x \rangle - i \langle S_y \rangle) \\ \frac{1}{\hbar}(\langle S_x \rangle + i \langle S_y \rangle) & \frac{1}{2} - \frac{\langle S_z \rangle}{\hbar} \end{pmatrix}$$

Discussion of the result:

- $\langle S_z\rangle = \langle S_x\rangle = \langle S_y\rangle = 0$ $\qquad \rho = \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix}$

  it is a completely incoherent statistical mixture $\frac{1}{2}|\uparrow\rangle\langle\uparrow| + \frac{1}{2}|\downarrow\rangle\langle\downarrow|$.

- $\langle S_z\rangle = \frac{\hbar}{2}$ and $\langle S_x\rangle = \langle S_y\rangle = 0$ pure state $\rho = |\uparrow\rangle\langle\uparrow|$.

  analogously $\langle S_z\rangle = -\frac{\hbar}{2}$ $\quad \langle S_x\rangle = \langle S_y\rangle = 0$ $\quad \rho = |\downarrow\rangle\langle\downarrow|$.

- Yet another simple example $\langle S_x\rangle = \frac{\hbar}{2}$ and $\langle S_y\rangle = \langle S_z\rangle = 0$

$$\rho = \begin{pmatrix} 1/2 & +1/2 \\ 1/2 & 1/2 \end{pmatrix} \qquad \rho = |x\uparrow\rangle\langle x\uparrow|$$

$$|x\uparrow\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle + |\downarrow\rangle\right)$$

$$\rho = \frac{1}{2}|\uparrow\rangle\langle\uparrow| + \frac{1}{2}|\downarrow\rangle\langle\uparrow| + \frac{1}{2}|\uparrow\rangle\langle\downarrow| + \frac{1}{2}|\downarrow\rangle\langle\downarrow| .$$

- But we can also work it out differently. Say we assume the statistical mixture

$$\rho = \frac{1}{2}|x\uparrow\rangle\langle x\uparrow| + \frac{1}{2}|y\downarrow\rangle\langle y\downarrow| = \frac{1}{2}\rho_{x\uparrow} + \frac{1}{2}\rho_{y\downarrow}$$

which are the expected $\langle S_i\rangle$?

$$\hat{\rho} = \frac{1}{4}\left(|\uparrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\uparrow| + |\uparrow\rangle\langle\downarrow| + |\downarrow\rangle\langle\downarrow|\right)$$

$$+ \frac{1}{4}\left(|\uparrow\rangle\langle\uparrow| - \frac{i}{1}|\downarrow\rangle\langle\uparrow| + i|\uparrow\rangle\langle\downarrow| + |\downarrow\rangle\langle\downarrow|\right)$$

$$= \begin{pmatrix} 1/2 & \frac{1}{4}+\frac{i}{4} \\ \frac{1}{4}-\frac{i}{4} & 1/2 \end{pmatrix}$$

Thus, for example, by measuring $\langle S_z\rangle$ alone, one could not distinguish: $\rho_{x\uparrow}$ from $\frac{1}{2}\rho_{x\uparrow} + \frac{1}{2}\rho_{y\downarrow}$.