

Abstract

Physical properties of many-particle quantum systems often do not depend on the wavefunction of the whole system but only on part of it, namely on the reduced density matrix of a few particles. Examples include the Pauli principle or the energy of systems with local interactions. In this proseminar, we will discuss the use of reduced density matrices in different parts of quantum physics, ranging from condensed matter systems and quantum chemistry to quantum information theory.

Organisation

Criteria for passing the module:

- Give a pedagogical presentation demonstrating solid understanding of the material.
- Be present at least 80% of the time.
- Hand in a written report of your talk in English.

Each presentation should last just less than 60 minutes. Students can either give a blackboard or a computer presentation.

Each student is assigned to a research assistant at the institute as a tutor for their talk.

The students should contact their tutor at least six weeks before their talk to discuss logistics. They should keep their tutor updated of their work at least once a week.

One week before their talk they are expected to have a draft of their report as well as a finished set of slides (or other notes) which they have to present to their tutor. The report should then be handed in two weeks after the talk.

Outline

Below you can find a list of all the talks. For each talk there is a brief description of the topic, a list of suggested items to be covered as well as some references; for more specific guidance and further references, please ask your tutor.

You are also encouraged to coordinate your talk with your neighbours where appropriate:

- Avoid excessive overlap between the talks;
- make references to other talks.
- Do not take away your successor's key points;
- rather prepare the audience for the topics to follow.

Time and Venue

The talks will be presented on Mondays, 9:45–12:45 in HIT K 51.

The below dates of the individual talks are tentative and subject to slight adjustments.

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A Basics

A1 The Set of Density Operators

Date: 5 Mar, 9:45 Student: Philipp Kammerlander Tutor: Mario Ziman

Description: The density operator is the mathematical answer to the following question: What is the most general state of a quantum system? In this sense it generalizes the concept of the wave function. In this proseminar we will follow two conceptually different paths (mixing of preparation procedures and ignorance of system's environment) leading to the same mathematical concept of density operator. We will analyze and interpret the spectral properties of density operators. Further we focus on the general structural properties of the set of density operators. We will identify the extremal states (i.e. those characterized by a unique decomposition) and exhibit the nonuniqueness of convex decompositions into pure states. We will define two measures of mixedness (purity and von Neumann purity) and discuss the concept of maximally mixed state. Introducing the Bloch representation we will investigate the geometry of state space, especially its boundary. Goals: Introduction of density operators and their elementary properties.

References:

- K.Zyczkowski, I.Bengtsson, Geometry of quantum states (Cambridge University Press, 2006)
- T.Heinosaari, M.Ziman, The Mathematical Language of Quantum Theory: From Uncertainty to Entanglement (Cambridge University Press, 2012)

A2 Time Evolution

Date: 5 Mar, 11:15 Student: Quintin Meier Tutor: Mario Ziman

Description: The Schrödinger equation is one of the postulates of quantum theory and determines the time evolution of pure quantum states (wave functions) of an isolated quantum systems. We will derive its equivalent for density operators known as von Neumann equation. We will show that the formal solution has the form of a one-parametric group of unitary conjugations for any time interval. Further we will study the evolution of a subsystem and introduce the idea of a quantum channel generalizing the unitary evolution along the same lines as density operators are generalizing the wave functions. To get a better insight into non-unitary dynamics we will illustrate some elementary examples of quantum channels. After that we will abstract the mathematical properties of quantum channels and formulate the Stinespring representation theorem. If time remains we will discuss the mathematical requirements standing behind the form of Schrödinger equation.

Goals: Introduction of von Neumann equation and framework of quantum channels.

References:

- H.P.Breuer, F.Petruccione, The theory of open quantum systems (Oxford University Press, 2002)
- M.Nielsen, I.Chuang, Quantum Information and quantum computation (Cambridge University Press, 2000)
- B.Simon, Quantum dynamics: From automorphism to Hamiltonian, Studies in Mathematical Physics, Essays in Honor of Valentine Bargmann (ed. E.H. Lieb, B. Simon and

B Quantum Information Theory

B1 Quantum Marginal Problem: Specific Results

Date: 12 Mar, 9:45 Student: Francisco Kim Tutor: Johan Aaberg

Description: The Quantum Marginal Problem asks for the compatibility of a set of reduced density matrices with a global quantum state. This problem is difficult in general (see next talk), but remarkable solutions have been obtained in a number of instances.

References:

- N. Linden, S. Popescu, W.K. Wootters, Almost Every Pure State of Three Qubits Is Completely Determined by Its Two-Particle Reduced Density Matrices, *Phys. Rev. Lett.* 89, 207901 (2002)
- N. Linden, S. Popescu, W.K. Wootters, The power of reduced quantum states, [arXiv: quant-ph/0207109](https://arxiv.org/abs/quant-ph/0207109)
- One-Qubit Reduced States of a Pure Many-Qubit State: Polygon Inequalities, A. Higuchi, A. Sudbery, and J. Szulc, *Phys. Rev. Lett.* 90, 107902 (2003)
- A. Klyachko, Quantum marginal problem and representations of the symmetric group, [arXiv: quant-ph/0409113](https://arxiv.org/abs/quant-ph/0409113)

B2 Quantum Marginal Problem: Computational Complexity

Date: 12 Mar, 11:15 Student: Gregor Kälin Tutor: Christopher Portman

Description: The quantum marginal problem, i.e. the problem of deciding whether a set of reduced density matrices is consistent with a global quantum state, is computationally difficult. More precisely, it is QMA-complete. QMA is the quantum analog of the classical complexity class NP and it is not believed that there exist efficient algorithms to solve QMA-complete problems.

References: The first reference is specific to the result to be discussed, the second is a general introduction to (quantum) complexity theory.

- Yi-Kai Liu, Consistency of Local Density Matrices is QMA-complete, [arXiv: quant-ph/0604166](https://arxiv.org/abs/quant-ph/0604166), Proceedings of RANDOM 2006.
- (Book) A. Yu Kitaev, A. H. Shen, M. N. Vyalıy, Classical and Quantum Computation (Graduate Studies in Mathematics), AMS.

B3 Entropy Inequalities

Date: 19 Mar, 9:45 Student: Dominik Gresch Tutor: Christopher Portman

Description: An entropy inequality is an inequality relating the von Neumann entropies of different parts of a quantum system. All known inequalities can be derived from a single inequality known as strong subadditivity, but it remains an open question whether this is the only inequality.

References: The first reference is a general one for strong subadditivity. The search for new inequalities has been started in the second reference and the third reference reports on the first progress in this question.

- (Book) Nielsen and Chuang, Quantum Computation and Information, Cambridge University Press.
- N. Pippenger, The inequalities of quantum information theory, IEEE Transactions on Information Theory, Vol. 49, 773 - 789 (2003)
- Noah Linden und Andreas Winter, A New Inequality for the von Neumann Entropy, Comm. Math. Phys. Vol. 259, 129-138 (2005)

B4 Entanglement

Date: 19 Mar, 11:15 Student: Felix Bischof Tutor: Frederic Dupuis

Description: Suppose we have a randomly-chosen quantum state over three systems A, B, and C. How likely is it that the reduced state on A and B will be entangled? In this project, we will show that if the state is random enough, the state on AB will, with very high probability, be in a subspace containing only highly entangled states.

References:

- R., P., M. and K. Horodecki, Quantum entanglement, Rev. Mod. Phys. 81, 865D942 (2009)
- Patrick Hayden, Debbie W. Leung, Andreas Winter, Aspects of generic entanglement, Comm. Math. Phys. Vol. 265, No. 1, pp. 95-117, 2006. [quant-ph/0407049](#)

B5 Quantum Coding

Date: 26 Mar, 9:45 Student: Ilario Giordanelli Tutor: Frederic Dupuis

Description: One important property of quantum mechanics is that, given any reduced density matrix, one can find a pure state on a larger Hilbert space compatible with it. In particular, if a state on AB is completely uncorrelated, then both A and B must be highly correlated with the purifying system. In this project, we will see how we can use this fact to perform the very counterintuitive task of transmitting information by destroying correlations.

References:

- Uhlmann's Theorem in M. A. Nielsen and I. L. Chuang, "Quantum computations and quantum information" (Cambridge University Press, Cambridge, 2000).
- Federic Dupuis, Mario Berta, Jürg Wullschleger, Renato Renner, The Decoupling Theorem [arXiv:1012.6044](#)

C Thermodynamics

C1 Thermal Equilibrium via Entanglement

Date: 26 Mar, 11:15 Student: Tileman Conring Tutor: Johan Aaberg

Description: In quantum mechanics a subsystem can be mixed although the total state is pure. This has been the starting point for several approaches to explain thermal equilibrium states.

References:

- J. Gemmer, M. Michel, and G. Mahler, "Quantum thermodynamics" (Springer-Verlag, Berlin, 2004).
- S. Goldstein, J. L. Lebowitz, R. Tumulka, and N. Zanghi, "Canonical typicality", *Physical Review Letters*, Vol. 96, 050403 (2006).
- S. Popescu, A. J. Short, and A. Winter, "Entanglement and the foundations of statistical mechanics", *Nature Physics*, Vol. 2, 754 (2006). (For more details, see arXiv: quant-ph/0511225.)
- S. Lloyd, "Excuse our ignorance", *Nature Physics*, Vol. 2, 727 (2006).

C2 Approaching Thermal Equilibrium

Date: 2 Apr, 9:45

Student: Selim Kangeldi

Tutor: Joe Renes

Description:

Many different arguments have been put forward to theoretically explain the tendency of physical systems to approach thermal equilibrium. For this particular project, the focus is on equilibration of typical states and the restriction to "realistic" observables.

References:

- N. Linden, S. Popescu, A. J. Short, and A. Winter, "Quantum mechanical evolution towards thermal equilibrium", *Physical Review E*, Vol. 79, 061103 (2009).
- P. Reimann, "Foundation of statistical mechanics under experimentally realistic conditions", *Physical Review Letters*, Vol. 101, 190403 (2008).
- P. Reimann, "Canonical thermalization", *New Journal of Physics*, Vol. 12, 055027 (2010).
- A. Riera, C. Gogolin, and J. Eisert, "Thermalization in nature and on a quantum computer", arxiv:1102.2389.
- A. J. Short, "Equilibration of quantum systems and subsystems", *New Journal of Physics*, Vol. 13, 053009 (2011).
- J. L. Lebowitz, "Statistical mechanics: A selective review of two central issues", *Reviews of Modern Physics*, Vol. 71, 5346 (1999).

C3 Jaynes' Principle

Date: 2 Apr, 11:15

Student: Thomas Karg

Tutor: Joe Renes

Description: Given a collection of expectation values, Jaynes' principle (also called the "maximum entropy principle") provides a method to infer the density operator (or probability distribution) of the system. This gives an alternative (but debated) foundation for statistical mechanics, and has been a popular tool also outside of physics.

References:

- E. T. Jaynes, "Information theory and statistical mechanics", *Physical Review*, Vol. 106, 620 (1957).

- E. T. Jaynes, "Information theory and statistical mechanics II", *Physical Review*, Vol. 108, 171 (1957).
- J. Uffink, "The constraint rule of the maximum entropy principle", *Studies in the History and Philosophy of Science*, Vol. 27, 47 (1996).

C4 NMR Quantum Computing

Date: 23 Apr, 9:45 Student: Lukas Hutmacher Tutor: Ludwig Klam

Description: It has been suggested that nuclear magnetic resonance (NMR) techniques could be used for quantum computing. In this approach each single molecule in a liquid works as a quantum computer. A much debated question is how the very mixed thermal states of these molecules can function as a substrate for quantum computing.

References:

- Section 7.7 "Nuclear magnetic resonance" in M. A. Nielsen and I. L. Chuang, "Quantum computations and quantum information" (Cambridge University Press, Cambridge, 2000).
- D. G. Cory, A. F. Fahmy, and T. F. Havel, "Ensemble quantum computing by NMR spectroscopy", *Proceedings of the National Academy of Sciences, USA*, Vol. 94, 1634 (1997).
- N. A. Gershenfeld and I. L. Chuang, "Bulk spin-resonance quantum computation", *Science*, Vol. 275, 350 (1997).
- E. Knill, I. Chuang, and R. Laflamme, "Effective pure states for bulk quantum computation", *Physical Review A*, Vol. 57, 3348 (1998).
- N. Linden and S. Popescu, *Physical Review Letters*, "Good dynamics versus bad kinematics: Is entanglement needed for quantum computation?", Vol. 87, 047901 (2001).

D Condensed Matter and Computational Physics

D1 Density Matrix Renormalization Group Method (DMRG)

Date: 23 Apr, 11:15 Student: Peter Strassmann Tutor: Philippe Corboz

Description: The Density Matrix Renormalization Group (DMRG) is the most powerful method for the simulation of one dimensional strongly-correlated quantum many-body systems. Its success lies in an efficient truncation of the Hilbert space, where the reduced density matrix of a subsystem plays the key role to identify the most relevant states.

References:

- S.R. White, *Phys. Rev. Lett.* 69, 2863 (1992).
- U. Schollwöck, *Rev. Mod. Phys.* 77, 259 (2005).
- I. Peschel, X. Wang, M. Kaulke, and K. Hallberg, *Density-Matrix Renormalization - A New Numerical Method in Physics: Lectures of a Seminar and Workshop Held at the Max-Planck-Institut Für Physik ... 18th, 1998*, Softcover reprint of hardcover 1st ed. 1999 ed. (Springer Berlin Heidelberg, 2010).

D2 Matrix product states (MPS) and projected entangled-pair states (PEPS)

Date: 30 Apr, 9:45 Student: Maximilian Voss Tutor: Philippe Corboz

Description: Matrix product states (MPS) enable an efficient representation of (quasi-) one-dimensional quantum-many body states, and form the class of variational states underlying the powerful DMRG method (see D1). Besides DMRG new algorithms have been developed directly in the language of MPS, e.g. for the imaginary- and real-time evolution of an MPS. Progress in Quantum Information Theory, in particular a better understanding of entanglement in quantum-many body states, led to generalization of MPS to two dimensions, called projected entangled-pair states (PEPS) which are able to reproduce the area law of the entanglement entropy in two dimensions.

References:

- U. Schollwöck, *Annals of Physics* 326, 96 (2011).
- F. Verstraete, V. Murg, and J.I. Cirac, *Advances in Physics* 57, 143 (2008).
- J. Eisert, M. Cramer, and M.B. Plenio, *Rev. Mod. Phys.* 82, 277 (2010).

E Fermionic Systems

E1 N-Representability Problem: Pauli Principle and Beyond

Date: 30 Apr, 11:15 Student: Dario Schöbi Tutor: Roger Colbeck

Description: The N-representability is the fermionic version of the quantum marginal problem: given a k-particle fermionic state, determine whether or not it arises as the reduced density matrix of an N-particle fermionic state. A well-known necessary condition for a one-particle density operator to be N-representable is Pauli's principle which in this formulation simply means that the largest eigenvalue of the one-particle density matrix is one (we use chemists notation where the trace of the one-particle density matrix equals N). Recently more such conditions have been discovered and are the topic of this talk. Good approximations to the set of two-particle N-representable density matrices can be obtained using semi-definite programming. This old idea has recently been going through a renaissance.

References:

- Coleman and Yukalov, *Reduced Density Matrices: Coulson's Challenge*, Lecture Notes in Chemistry, Springer, 2000
- Borland and Dennis, The conditions on the one-matrix for three-body fermion wavefunctions with one-rank equal to six, *J. Phys. B: At. Mol. Phys.* vol. 5 page 7 (1972)
- Alexander A Klyachko, Quantum marginal problem and N-representability, *J. Phys.: Conf. Ser.* 36 72 (2006)

E2 N-Representability Problem: Semidefinite Constraints

Date: 7 May, 9:45 Student: Abas Jusufi Tutor: Roger Colbeck

Description: Determining whether a two-particle density operator is N-representable is an

important problem in quantum chemistry as its efficient solution would allow the efficient computation of ground state energies in atoms and molecules. It turns out, however, that the problem is computationally difficult (QMA hard).

References:

- Coleman, Yukalov, *Reduced Density Matrices: Coulson's Challenge*, Lecture Notes in Chemistry, Springer, 2000
- Fukuda et al, *Mathematical Programming*, Volume 109, Numbers 2-3, 553-580 (2007) Large-scale semidefinite programs in electronic structure calculation

E3 Fermionic Density Functional Theory

Date: 7 May, 11:15 Student: Fabio D'Ambrosi

Tutor: Lei Wang

Description: Density functional theory treats ground state density as a central quantity of many-body quantum mechanics. By balancing both accuracy and efficiency, it finds enormous applications in physics, chemistry and biophysics. This talk should focus on theoretical foundations of density functional theory. The students is also encouraged to look into (time-dependent, finite-temperature, density-matrix, lattice etc) generalizations of density functional theory.

Goals: Proof Hohenberg-Hohn theorem, introduce Kohn-Sham system, discuss use and abuse of density functional theory.

References:

- P. Hohenberg and W. Kohn, "Inhomogeneous electron gas", *Physical Review*, Vol. 136, B864 (1964).
- W. Kohn and L. J. Sham, "Self-consistent equations including exchange and correlation effects", *Physical Review*, Vol. 140, A1133 (1965).
- K. Capelle, "A bird's-eye view of density-functional theory", arXiv:cond-mat/0211443 (2006).
- A. S. Bamzai and B. M. Deb, "The role of single-particle density in chemistry", *Reviews of Modern Physics*, Vol. 53, 95 (1981).
- M. Levy, "Universal variational functionals of electron densities, first-order density matrices, and natural spin-orbitals and solution of the v-representability problem", *Proceedings of the national Academy of Sciences, USA*, Vol. 76, 6062 (1979).

F Bosonic Systems

F1 Mean Field Theory: Explicit Derivations

Date: 14 May, 9:45 Student: Ursin Solèr

Tutor: Marcello Portas

Description: The talk should give an overview about mean-field constructions in theoretical physics, their applicability and weaknesses. Special focus is laid on spin systems and Bose-Einstein condensates. The talk should cover the physical arguments why and when mean-field techniques are applicable for such systems, as well as giving an overview about heuristic arguments for condensation.

References:

- (classical mean-field theory) T. Dorlas, Statistical Mechanics: Fundamentals and Model Solutions
- (Bose-condensation) T. Dorlas, Statistical Mechanics: Fundamentals and Model Solutions and Chapter 1-2 of the book "The mathematics of the bose gas and its condensation" by Elliott H. Lieb, Robert Seiringer, Jan Philip Solovej and Jakob Yngvason.

F2 Mean Field Theory: General Results

Date: 14 May, 11:15 Student: Maximilian Häfliger

Tutor: Volkher Scholz

Description: This talk should focus on the rigorous mean-field theory for spin systems due to R.F. Werner and coworkers. It is based on algebraic consideration involving symmetries of the system, and leads to one approach to describe the transition to classicality of quantum many body systems, based on the dynamical rules for the reduced density matrices.

References: G. A. Raggio and R. F. Werner, Quantum statistical mechanics of general mean field systems. Helv. Phys. Acta 62(1989) 980-1003

F3 Bose-Einstein Condensates and the Gross-Pitaevskii Equation

Date: 21 May, 9:45 Student: Arne Hansen

Tutor: Gang Zhon

Description: The ground state energy as well as the ground state wave function of a Bose gas subject to an external potential, like an optical trap, can be calculated from a non-linear functional called the Gross-Pitaevskii functional. This talk should explain and verify the statement, as well as giving an outlook on the dynamics of Bose-Einstein condensates.

References: Chapter 1,6 of "The mathematics of the bose gas and its condensation" by Elliott H. Lieb, Robert Seiringer, Jan Philip Solovej and Jakob Yngvason.

G Open Systems

G1 Master Equation

Date: 21 May, 11:15 Student: Claudio Paganini

Tutor: Martin Fraas

Description: If the collection of dynamical maps in a physical system forms a semi-group of trace preserving completely positive maps, one can show (with some additional assumption on continuity) that these satisfy a differential equation of a special form; the Lindblad-Kossakowski master equation.

References:

- G. Lindblad, "On the generators of quantum dynamical semigroups", Communications in Mathematical Physics, Vol. 48, 119 (1979).
- A. Kossakowski, "On quantum statistical mechanics of non-Hamiltonian systems", Reports in Mathematical Physics, Vol. 3, 247 (1972).

- V. Gorini, A. Kossakowski, and E. C. G. Sudarshan, "Completely positive dynamical semigroups of N-level systems", *Journal of mathematical physics*, Vol. 17, 821 (1976).
- Section 3.2 "Quantum Markov processes" in "The theory of open quantum systems" by Heinz-Peter Breuer, and Francesco Petruccione (Oxford Publishers, 2007).

Starting from explicit models of a system interacting with a heat-bath, there exists many different techniques to derive (often approximate) master equations for the evolution of the reduced density operator of the system. Two common examples are:

- The Born-markov approximation. See, Section 3.3 "Microscopic derivations" (and forward in sec. 3 for examples) in "The theory of open quantum systems" by Heinz-Peter Breuer and Francesco Petruccione (Oxford Publishers, 2007).
- The Projection Operator Techniques. See Section 9 "Projection Operator Techniques" in "The theory of open quantum systems" by Heinz-Peter Breuer and Francesco Petruccione (Oxford Publishers, 2007).

For this project one could focus on one particular technique, go through its derivation, and maybe apply it to some simple example.

G2 Unravelling Master Equations

Date: 28 May, 9:45 Student: Levy Jäger

Tutor: Martin Fraas

Description: In an "unravelling" of a master equation (there exists several versions) the solution of a master equation is obtained as an average over many stochastically evolved pure states. Three common examples are:

- Operational description of continuous measurements in quantum optics. See the book of E. B. Davies (1976).
- Quantum jump approach to the photon counting statistic. See Cohen-Tannoudji and Dalibard (1986) or a review by Plenio and Knight (1998).
- The quantum state diffusion model. See Gisin and Percival (1992). (This version involve concept of stochastic differential equations.)

The student is asked to pick one of these approaches, to explain it's physical content and to connect it to the Lindblad master equation.

References:

- E. B. Davies, "Quantum theory of open systems", Academic Press, London (1976).
- C. Cohan-Tannoudji and J. Dalibard, "Single atom laser spectroscopy. Looking for dark periods in fluorescence light", *Europhysics letters*, Vol 1, 441 (1986).
- M. B. Plenio and P. L. Knight, "The quantum-jump approach to dissipative dynamics in quantum optics", *Review of Modern Physics*, Vol. 70, 101 (1998).
- N. Gisin and I. C. Percival, "The quantum-state diffusion model applied to open systems", *Journal of Physics A: Mathematical and General* , Vol. 25, 5677 (1992).