

Contents

| | | |
|----------|---|---------------|
| 1 | A primer on electron transport | <i>page</i> 1 |
| 1.1 | Nanoscale systems | 1 |
| 1.2 | Generating currents | 3 |
| 1.2.1 | Finite versus infinite systems | 8 |
| 1.2.2 | Electron sources | 9 |
| 1.2.3 | Intrinsic nature of the transport problem | 10 |
| 1.3 | Measuring currents | 11 |
| 1.3.1 | Microscopic states | 12 |
| 1.3.2 | The current operator | 13 |
| 1.3.3 | The measurement process | 16 |
| 1.3.4 | Complete measurement and pure states | 17 |
| 1.4 | The statistical operator and macro-states | 19 |
| 1.4.1 | Pure and mixed states | 21 |
| 1.4.2 | Quantum correlations | 22 |
| 1.4.3 | Time evolution of the statistical operator | 23 |
| 1.4.4 | Random or partially specified Hamiltonians | 24 |
| 1.4.5 | Open quantum systems | 25 |
| 1.4.6 | Equilibrium statistical operators | 29 |
| 1.5 | Current measurement and statistical operator truncation | 32 |
| 1.6 | One current, different viewpoints | 34 |
| | Summary and open questions | 36 |
| | Exercises | 36 |
| 2 | Drude model, Kubo formalism and Boltzmann equation | 39 |
| 2.1 | Drude model | 39 |
| 2.2 | Resistance, coherent and incoherent transport | 42 |
| 2.2.1 | Relaxation vs. dephasing | 44 |

| | | |
|----------|--|-----|
| viii | <i>Contents</i> | |
| | 2.2.2 Mean-free path | 48 |
| | 2.2.3 The meaning of momentum relaxation time | 49 |
| 2.3 | Kubo formalism | 50 |
| | 2.3.1 The current-current response function | 55 |
| | 2.3.2 The use of Density-Functional Theory in the Kubo approach | 57 |
| | 2.3.3 The fluctuation-dissipation theorem | 60 |
| | 2.3.4 Ohmic vs. ballistic regimes | 66 |
| 2.4 | Chemical, electrochemical and electrostatic potentials | 68 |
| 2.5 | Drift-diffusion equations | 72 |
| | 2.5.1 Diffusion coefficient of an ideal electron gas in the non-degenerate limit | 73 |
| | 2.5.2 Generalization to spin-dependent transport | 75 |
| 2.6 | Distribution functions | 77 |
| 2.7 | Boltzmann equation | 79 |
| | 2.7.1 Approach to local equilibrium | 82 |
| 2.8 | Entropy, loss of information, and macroscopic irreversibility | 83 |
| | 2.8.1 The classical statistical entropy | 85 |
| | 2.8.2 Quantum statistical entropy | 86 |
| | 2.8.3 Information content of the N - and one-particle statistical operators | 89 |
| | 2.8.4 Entropy of open quantum systems | 90 |
| | 2.8.5 Loss of information in the Kubo formalism | 91 |
| | 2.8.6 Loss of information with stochastic Hamiltonians | 92 |
| | 2.8.7 Entropy associated with the measurement of currents | 93 |
| | Summary and open questions | 94 |
| | Exercises | 95 |
| 3 | Landauer approach | 101 |
| | 3.1 Formulation of the problem | 102 |
| | 3.2 Local resistivity dipoles and the “field response” | 113 |
| | 3.3 Conduction from transmission | 115 |
| | 3.3.1 Scattering boundary conditions | 115 |
| | 3.3.2 Transmission and reflection probabilities | 119 |
| | 3.3.3 Total current | 123 |
| | 3.3.4 Two-probe conductance | 128 |
| | 3.4 The Lippmann–Schwinger equation | 132 |
| | 3.4.1 Time-dependent Lippmann–Schwinger equation | 132 |
| | 3.4.2 Time-independent Lippmann–Schwinger equation | 140 |
| | 3.5 Green’s functions and self-energy | 145 |

| <i>Contents</i> | | ix |
|-----------------|--|------------|
| 3.5.1 | Relation to scattering theory | 154 |
| 3.6 | The \mathcal{S} matrix | 159 |
| 3.6.1 | Relation between the total Green's function and the \mathcal{S} matrix | 162 |
| 3.7 | The transfer matrix | 167 |
| 3.7.1 | Coherent scattering of two resistors in series | 169 |
| 3.7.2 | Incoherent scattering of two resistors in series | 171 |
| 3.7.3 | Relation between the conductance and the transfer matrix | 173 |
| 3.7.4 | Localization, ohmic and ballistic regimes | 174 |
| 3.8 | Four-probe conductance in the non-invasive limit | 178 |
| 3.8.1 | Single-channel case | 179 |
| 3.8.2 | Geometrical "dilution" | 181 |
| 3.8.3 | Multi-channel case | 182 |
| 3.9 | Multi-probe conductance in the invasive limit | 185 |
| 3.9.1 | Floating probes and dephasing | 187 |
| 3.10 | Generalization to spin-dependent transport | 190 |
| 3.10.1 | Spin-dependent transmission functions | 194 |
| 3.10.2 | Multi-probe conductance in the presence of a magnetic field | 195 |
| 3.10.3 | Local resistivity spin dipoles and dynamical effects | 196 |
| 3.11 | The use of Density-Functional Theory in the Landauer approach | 198 |
| | Summary and open questions | 202 |
| | Exercises | 203 |
| 4 | Non-equilibrium Green's function formalism | 209 |
| 4.1 | Formulation of the problem | 211 |
| 4.1.1 | Contour ordering | 215 |
| 4.2 | Equilibrium Green's functions | 217 |
| 4.2.1 | Time-ordered Green's functions | 218 |
| 4.2.2 | Dyson's equation for interacting particles | 221 |
| 4.2.3 | More Green's functions | 223 |
| 4.2.4 | The spectral function | 225 |
| 4.3 | Contour-ordered Green's functions | 231 |
| 4.3.1 | Equations of motion for non-equilibrium Green's functions | 233 |
| 4.4 | Application to steady-state transport | 236 |
| 4.5 | Coulomb blockade | 244 |
| 4.6 | Quantum kinetic equations | 250 |

| | | |
|----------|---|-----|
| x | <i>Contents</i> | |
| | Summary and open questions | 255 |
| | Exercises | 257 |
| 5 | Noise | 258 |
| | 5.1 The moments of the current | 261 |
| | 5.2 Shot noise | 263 |
| | 5.2.1 The classical (Poisson) limit | 264 |
| | 5.2.2 Quantum theory of shot noise | 266 |
| | 5.3 Counting statistics | 274 |
| | 5.4 Thermal noise | 275 |
| | Summary and open questions | 277 |
| | Exercises | 277 |
| 6 | Electron-ion interaction | 280 |
| | 6.1 The many-body electron-ion Hamiltonian | 281 |
| | 6.1.1 The adiabatic approximation for a current-carrying system | 282 |
| | 6.1.2 The phonon subsystem | 284 |
| | 6.1.3 Electron-phonon coupling in the presence of current | 288 |
| | 6.2 Inelastic current | 290 |
| | 6.2.1 Inelastic current from standard perturbation theory | 291 |
| | 6.2.2 Inelastic current from the NEGF | 296 |
| | 6.3 Local ionic heating | 312 |
| | 6.3.1 Lattice heat conduction | 319 |
| | 6.4 Thermopower | 323 |
| | 6.5 Current-induced forces | 328 |
| | 6.5.1 Elastic vs. inelastic contribution to electro-migration | 328 |
| | 6.5.2 One force, different definitions | 330 |
| | 6.5.3 Local resistivity dipoles and the force sign | 333 |
| | 6.5.4 Forces at equilibrium | 333 |
| | 6.5.5 Forces out of equilibrium | 335 |
| | 6.5.6 Are current-induced forces conservative? | 340 |
| | 6.6 Local ionic heating vs. current-induced forces | 343 |
| | Summary and open questions | 344 |
| | Exercises | 344 |
| 7 | The micro-canonical picture of transport | 346 |
| | 7.1 Formulation of the problem | 347 |
| | 7.1.1 Transport from a finite-system point of view | 347 |
| | 7.1.2 Initial conditions and dynamics | 349 |
| | 7.2 Electrical current theorems within dynamical DFTs | 351 |
| | 7.2.1 Closed and finite quantum systems in a pure state | 351 |

| <i>Contents</i> | | xi |
|-------------------|---|------------|
| 7.2.2 | Closed quantum systems in a pure state with arbitrary boundary conditions | 353 |
| 7.2.3 | Current in open quantum systems | 354 |
| 7.2.4 | Closure of the BBGKY hierarchy | 356 |
| 7.2.5 | Functional approximations and loss of information | 357 |
| 7.3 | Transient dynamics | 358 |
| 7.4 | Properties of quasi-steady states | 360 |
| 7.4.1 | Variational definition of quasi-steady states | 360 |
| 7.4.2 | Dependence of quasi-steady states on initial conditions | 364 |
| 7.5 | A non-equilibrium entropy principle | 365 |
| 7.6 | Approach to steady state in nanoscale systems | 369 |
| 7.7 | Definition of conductance in the micro-canonical picture | 374 |
| | Summary and open questions | 375 |
| 8 | Hydrodynamics of the electron liquid | 376 |
| 8.1 | The Madelung equations for a single particle | 378 |
| 8.2 | Hydrodynamic form of the Schrödinger equation | 380 |
| 8.2.1 | Quantum Navier–Stokes equations | 382 |
| 8.3 | Conductance quantization from hydrodynamics | 388 |
| 8.4 | Viscosity from Time-Dependent Current Density-Functional Theory | 391 |
| 8.4.1 | Functional approximation, loss of information, and dissipative dynamics | 394 |
| 8.4.2 | Effect of viscosity on resistance | 395 |
| 8.5 | Turbulent transport | 397 |
| 8.6 | Local electron heating | 403 |
| 8.6.1 | Electron heat conduction | 405 |
| 8.6.2 | Hydrodynamics of heat transfer | 406 |
| 8.6.3 | Effect of local electron heating on ionic heating | 410 |
| | Summary and open questions | 412 |
| | Exercises | 413 |
| Appendices | | |
| <i>Appendix A</i> | A primer on second quantization | 415 |
| <i>Appendix B</i> | The quantum BBGKY hierarchy | 420 |
| <i>Appendix C</i> | The Lindblad equation | 423 |
| C.1 | The Lindblad theorem | 424 |
| C.2 | Derivation of the Lindblad equation | 426 |
| C.3 | Steady-state solutions | 430 |

| | |
|---|-----|
| Appendix D Ground-state Density-Functional Theory | 431 |
| D.1 The Hohenberg–Kohn theorem | 431 |
| D.2 The Kohn–Sham equations | 432 |
| D.3 Generalization to grand-canonical equilibrium | 434 |
| D.4 The local density approximation and beyond | 434 |
| Appendix E Time-Dependent DFT | 436 |
| E.1 The Runge–Gross theorem | 436 |
| E.2 The time-dependent Kohn–Sham equations | 437 |
| E.3 The adiabatic local density approximation | 437 |
| Appendix F Time-Dependent Current DFT | 439 |
| F.1 The current density as the main variable | 439 |
| F.2 The exchange-correlation electric field | 440 |
| F.3 Approximate formulas for the viscosity | 442 |
| Appendix G Stochastic Time-Dependent Current DFT | 444 |
| G.1 The stochastic Schrödinger equation | 444 |
| G.2 Derivation of the quantum master equation | 446 |
| G.3 The theorem of Stochastic TD-CDFT | 449 |
| Appendix H Inelastic corrections to current and shot noise | 451 |
| Appendix I Hydrodynamic form of the Schrödinger equation | 454 |
| Appendix J Equation of motion for the stress tensor | 458 |
| Appendix K Cut-off of the viscosity divergence | 461 |
| Appendix L Bernoulli’s equation | 463 |
| <i>References</i> | 464 |
| <i>Index</i> | 470 |