

# Contents

## Part I Introduction

<b>1</b>	<b>Quantum Many-Particle Systems out of Equilibrium</b>	3
1.1	Overview on Computational Approaches	5
1.2	Many-Body Interactions in Inhomogeneous Quantum Systems	7
1.3	Correlations	9

## Part II Theory

<b>2</b>	<b>Nonequilibrium Green's Functions</b>	15
2.1	Introduction	16
2.1.1	Keldysh Contour	17
2.1.2	One-Particle Nonequilibrium Green's Function	19
2.2	Equations of Motion	22
2.2.1	Keldysh-Kadanoff-Baym Equations	24
2.2.2	Equilibrium Limit. Dyson Equation	26
2.3	Many-Body Approximations	28
2.3.1	Requirements for a Conserving Scheme	29
2.3.2	Perturbation Expansions	29
2.4	Quantum Kinetic Equations for Single-Time Quantities	33
2.4.1	The Reconstruction Problem for the One-Particle Green's Function	34
2.4.2	The Generalized Kadanoff-Baym Ansatz	37

## Part III Computational Methods

<b>3</b>	<b>Representations of the Nonequilibrium Green's Function</b>	41
3.1	Numerical Resources	41
3.1.1	Homogeneous Systems. A Brief Outline	41
3.1.2	Inhomogeneous Systems. Computer Memory as Limiting Factor	44
3.2	Grid versus Basis Representations for Inhomogeneous Systems	44

3.3	An Efficient Solution: The Finite Element-Discrete Variable Representation . . . . .	47
3.3.1	General Idea and Background . . . . .	47
3.3.2	Construction of the FE-DVR Basis . . . . .	48
3.3.3	Matrix Elements of Relevant Energies . . . . .	51
3.3.4	First- and Second-Order Self-energies . . . . .	53
<b>4</b>	<b>Computation of Equilibrium States and Time-Propagation . . . . .</b>	<b>55</b>
4.1	Preparing the Initial State: Ground State or Equilibrium . . . . .	55
4.1.1	Time or Frequency Space? . . . . .	56
4.1.2	Solution of the Dyson Equation in $\tau$ -Space . . . . .	58
4.2	Nonequilibrium . . . . .	60
4.2.1	Two-Time Propagation Method . . . . .	60
4.2.2	Parallelization Strategies . . . . .	63
4.2.3	Single-Time Propagation using the GKBA . . . . .	68
 <b>Part IV Applications for Inhomogeneous Systems</b>		
<b>5</b>	<b>Lattice Systems . . . . .</b>	<b>75</b>
5.1	Overview . . . . .	76
5.2	A Basic Example . . . . .	77
5.2.1	Dynamics Following a Non-Perturbative Excitation . . . . .	78
5.2.2	Absorption Spectrum in Second Born Approximation . . . . .	80
<b>6</b>	<b>Non-Lattice Systems . . . . .</b>	<b>83</b>
6.1	Small Atoms and Molecules. Ground State Properties and Response to External Fields . . . . .	83
6.1.1	Model-Like Treatment . . . . .	84
6.1.2	3D Atoms and Molecules . . . . .	94
6.2	Few-Electron Quantum Dots and Wells . . . . .	96
6.2.1	Correlation Effects in the Optical Absorption Spectra . . . . .	98
6.2.2	Electronic Double Excitations from the Kadanoff-Baym Equations . . . . .	100
<b>7</b>	<b>Conclusion and Outlook . . . . .</b>	<b>105</b>
7.1	Summary . . . . .	105
7.2	Prospects for Future Applications . . . . .	106
<b>Appendix A Second Quantization . . . . .</b>		<b>109</b>
A.1	Symmetry of Many-Body States . . . . .	109
A.2	Occupation Number Representation . . . . .	110
A.3	Particle Creation and Annihilation in Fock Space . . . . .	111
A.4	General Form of Operators . . . . .	112
<b>Appendix B Perturbation Expansion. Supplements . . . . .</b>		<b>115</b>
B.1	Derivative of a Contour-Ordered Product . . . . .	115
B.2	Equations for $\Sigma^{(1)}$ and $\delta G^{(1)}/\delta v^{(1)}$ in Terms of $\delta \Sigma^{(1)}/\delta v^{(1)}$ . . . . .	117
<b>References . . . . .</b>		<b>119</b>
<b>Index . . . . .</b>		<b>129</b>

Nonequilibrium Green's Functions Approach to  
Inhomogeneous Systems

Balzer, K.; Bonitz, M.

2013, XII, 130 p. 31 illus., Softcover

ISBN: 978-3-642-35081-8