

# Contents

<b>1</b>	<b>Introduction</b>	<b>11</b>
<b>2</b>	<b>Methods</b>	<b>19</b>
2.1	Basic working principle of (Quantum) Monte Carlo . . . . .	21
2.2	Stochastic Series Expansion: general framework . . . . .	22
2.3	Updates . . . . .	25
2.3.1	Diagonal update . . . . .	25
2.3.2	Loop update . . . . .	29
2.3.3	Directed loop and generalization to spin $S$ . . . . .	30
2.4	Observables . . . . .	34
2.4.1	Static quantities . . . . .	34
2.4.2	Dynamic quantities . . . . .	37
2.4.3	Errors . . . . .	44
2.5	Maximum Entropy . . . . .	46
2.5.1	The continuation problem . . . . .	46
2.5.2	Singular value decomposition . . . . .	49
2.5.3	Regularization – the Maximum Entropy formalism . . . . .	51
2.5.4	Meshkov-Algorithm . . . . .	58
2.5.5	Bryan-Algorithm . . . . .	61
2.5.6	Conclusion . . . . .	63
<b>3</b>	<b>Static properties of low dimensional quantum magnets</b>	<b>65</b>

3.1	Spin $S$ chains – searching the classical limit . . . . .	67
3.1.1	Magnetic susceptibilities . . . . .	68
3.1.2	Padé-fits . . . . .	70
3.1.3	Conclusion . . . . .	73
3.2	Spin $S=1$ ladder system . . . . .	74
3.2.1	Magnetic susceptibility . . . . .	75
3.2.2	High-field magnetization . . . . .	79
3.2.3	Conclusion . . . . .	83
3.3	Spin $S$ grid systems . . . . .	84
3.3.1	The effect of center-spin coupling . . . . .	84
3.3.2	The effect of single-ion anisotropy . . . . .	87
3.3.3	Comparison to experimental data . . . . .	92
3.3.4	Conclusion . . . . .	94
<b>4</b>	<b>Dynamic properties of 1D quantum magnets</b>	<b>95</b>
4.1	Dynamic structure factors of the spin $1/2$ Heisenberg chain . . . . .	99
4.1.1	Longitudinal dynamic structure factor $S^{zz}(q, \omega)$ . . . . .	99
4.1.2	Transverse dynamic structure factor $S^{xx}(q, \omega)$ . . . . .	106
4.1.3	$T_1$ -relaxation rate of the spin $1/2$ Heisenberg chain . . . . .	110
4.1.4	Sum rules . . . . .	116
4.1.5	Conclusion . . . . .	118
4.2	Dynamic structure factors of the Haldane chain . . . . .	119
4.2.1	Temperature dependence of the transverse DSF . . . . .	119
4.2.2	Temperature dependence of the gap $\Delta(T)$ . . . . .	121
4.2.3	Low- $q$ behavior . . . . .	122
4.2.4	Field dependence of the transverse DSF . . . . .	124
4.2.5	NMR rates . . . . .	128
4.2.6	Sum rules . . . . .	131
4.2.7	Conclusion . . . . .	132

4.3 Hydrodynamic limit for the spin dynamics of the Heisenberg chain . . . . .	134
<b>5 Conclusion</b>	<b>143</b>
<b>Bibliography</b>	<b>149</b>
<b>The very last lines ...</b>	<b>163</b>