

CONTENTS

1	MOTIVATION	1
1.1	Historical overview	2
1.2	Shortcoming of the existing methods	5
2	NUMERICAL MODELLING	7
2.1	Basic definitions	7
2.2	Reduction to first-order systems	8
2.3	Fast Fourier transform	9
2.4	Matrix exponentials	11
2.4.1	Simplest cases	11
2.4.2	Scaling and squaring	12
2.4.3	Approximation in the Krylov subspace	12
3	COMPOSITION AND SPLITTING METHODS	15
3.1	Autonomous case	15
3.1.1	Composition of methods	15
3.1.2	System splitting	17
3.2	Time-dependent case	18
3.3	Order conditions	19
3.3.1	Baker–Campbell–Hausdorff formula	19
3.3.2	Order conditions via BCH	20
4	MAGNUS EXPANSION-BASED INTEGRATORS	23
4.1	Lie groups and Lie algebras	23
4.1.1	Lie groups	23
4.1.2	Lie algebras	23
4.1.2.1	Matrix Lie groups and their algebras . .	24
4.1.2.2	Lie algebra bases and BCH formula . .	25
4.2	Magnus expansion	25
4.2.1	Existence and properties	26
4.3	Application to the construction of integrators	28
4.3.1	Approximation with moment integrals	28
4.3.2	Magnus expansion in terms of generators	31
5	SCHRÖDINGER EQUATION	35
5.1	Lie algebra	37
5.2	Fourth-order methods	38
5.3	Sixth-order methods	41
5.4	Eighth-order methods	43
5.5	Numerical example	45
5.6	Conclusions	47

6 HILL AND WAVE EQUATION	51
6.1 Lie algebra	53
6.1.1 Time-dependent case	53
6.1.2 Half-autonomous case	55
6.2 Hill equation	56
6.3 Time-dependent wave equation	58
6.3.1 A general sixth-order method without commutators	59
6.3.2 Methods with modified potentials	61
6.3.2.1 Fourth-order methods	63
6.3.2.2 Sixth-order methods	65
6.4 Numerical examples	70
6.4.1 Mathieu equation	71
6.4.2 Hill equation	73
6.4.3 Wave equation	79
6.4.4 Klein–Gordon–Fock equation	79
6.5 Conclusions	80
7 NON-LINEAR CASE: KEPLER PROBLEM	83
7.1 Lie derivatives and Poisson brackets	84
7.2 Magnus-based methods for non-linear problems	86
7.3 Numerical examples	89
7.4 Conclusions	91
8 CONCLUSION	95
BIBLIOGRAPHY	97