

Contents

Preface	v
I Introduction	1
1 Schrödinger equation	1
2 Numerical schemes	3
2.1 Free Schrödinger equation	3
2.2 Potential part	4
2.3 Splitting schemes	4
2.4 Practical implementation	5
2.5 Semi-implicit schemes	8
3 Examples	9
3.1 Solitary waves	9
3.2 Linear equations	13
3.3 NLS in dimension 1: resonances and aliasing	16
3.4 Energy cascades in dimension 2	19
4 Objectives	23
II Finite dimensional backward error analysis	25
1 Hamiltonian ODEs	25
1.1 Definitions and basic properties	25
1.2 Expansion of the flow	28
2 Numerical integrators	29
3 Backward analysis for splitting methods	31
3.1 Setting of the problem	31
3.2 Baker–Campbell–Hausdorff formula	32
3.3 Recursive equations	35
III Infinite dimensional and semi-discrete Hamiltonian flow	39
1 NLS in Fourier space	40
2 Function spaces	42
3 Polynomials and vector fields	44
4 Local existence of the flow	49
5 Cases of global existence	53
6 Semi-discrete flow	56
IV Convergence results	60
1 Splitting methods and Lie derivatives	60
2 Convergence of the Lie splitting methods	62

3	Filtered splitting schemes	67
4	Space approximation	71
5	Fully discrete splitting method	74
V	Modified energy in the linear case	77
1	Operators, flow and splitting methods	77
1.1	Operators	77
1.2	Linear flow	80
1.3	Splitting methods	81
2	Formal series	81
3	Analytic estimates	83
4	Properties of the modified equation	85
5	Fully discrete splitting method	89
6	Resonance analysis	94
VI	Modified energy in the semi-linear case	97
1	Recursive equations	98
2	Construction of the modified energy	100
2.1	First terms	100
2.2	Iterative construction	102
3	Backward error analysis result	103
4	Fully discrete scheme	108
VII	Introduction to long time analysis	114
1	Resonant system	115
1.1	An approximation result	115
1.2	The resonance modulus	117
2	The one-dimensional case	118
2.1	Long time preservation of the actions	118
2.2	Aliasing and numerical resonances in dimension one	119
2.3	Fully discrete schemes	122
3	The case of dimension two	126
3.1	Energy cascades	126
3.2	Simulating energy cascades	132
	Bibliography	133
	Index	137