

Contents

1	Wave-Packet Dynamics: The Free-Particle Physics	1
1.1	Introduction	1
1.2	Propagation and Spreading	3
1.3	Dynamics on a Complex Configuration Space	9
1.4	Quantum Diffraction	12
1.5	Nonlocality and the Semiclassical Approach	18
1.6	Dissipation and Localization	20
1.6.1	Free Motion	20
1.6.2	Accelerated Motion and Limit Speeds	23
1.7	Stochastic Wave-Packet Dynamics	25
1.7.1	High Temperature Limit	25
1.7.2	Low and Zero Temperature Limit	27
1.8	Quantum Zeno and Anti-Zeno Effects	29
1.8.1	Projective Measurements	29
1.8.2	Thermal (Stochastic) Dynamics	38
1.9	Quantum Stochastic Trajectories and Weak Measurements	42
	References	44
2	Quantum Interference and Superposition	49
2.1	Introduction	49
2.2	Superposition Principle and Interference Dynamics	51
2.3	Interference and Effective Dynamic Potentials	58
2.4	Analogy Between Collisions and Wave-Packet Interference	64
2.5	Interference in a Complex Configuration Space	69
2.6	Young's Two-Slit Experiment	73
2.6.1	Interference and Boundary Effects	73
2.6.2	Realistic Two-Slit Diffraction	75
2.6.3	Decoherence and Contextuality	81
2.7	Dissipation Effects	87
2.8	Quantum Stochastic Trajectories. Schrödinger Cat States	90
	References	91

3	Interference and Interferometry	97
3.1	Introduction	97
3.2	Diffraction by Periodic Grating	99
3.3	Matter-Wave Mach-Zehnder Interferometry	105
3.3.1	General Aspects	105
3.3.2	The Ronchi Grating Model	108
3.3.3	The Gaussian Model	111
3.4	Near Field and Talbot Effect	115
3.5	Surfaces, Gratings and the Classical Limit	127
	References	129
4	Bound System Dynamics	135
4.1	Introduction	135
4.2	Eigenstates and Stationarity	138
4.2.1	Bohmian Stationarity	138
4.2.2	The Harmonic Oscillator	139
4.2.3	Eigenstate Superpositions and Motion	140
4.2.4	Phase Topology and Motion	142
4.2.5	Other Solutions to the Stationarity Problem	143
4.3	The Particle in the Box	145
4.3.1	Recurrences	145
4.3.2	Aspects of Classicality	147
4.4	Fractal Bohmian Mechanics	149
4.4.1	Quantum Fractals	149
4.4.2	Quantum Fractal Trajectories	152
4.5	Coherent Wave Packets	156
4.5.1	Real Configuration Space Dynamics	156
4.5.2	Complex Configuration Space Dynamics	159
4.6	The Quantum van der Pol Oscillator	161
4.7	Dissipative Dynamics	165
	References	169
5	Tunneling Dynamics	173
5.1	Introduction	173
5.2	The Role of Initial Conditions	174
5.3	Reactivity and Interference	178
5.3.1	Single Trajectory Dynamics	179
5.3.2	Statistical Ensemble Dynamics	181
5.4	Strong-Field Ionization: Time-Dependent Tunneling	184
5.5	Tunneling in Two-Level Chiral Systems. A Canonical Formalism	191
5.5.1	Isolated Two-Level Chiral Systems	192
5.5.2	Non-isolated Two-Level Chiral Systems	193
5.5.3	Thermodynamics from Stochastic Dynamics	196
5.6	Tunneling in Periodic Surfaces	201
	References	208

6	Atom Scattering from Periodic Surfaces	213
6.1	Introduction	213
6.2	Quantum Elastic Scattering. Background	214
6.3	Quantum Trajectories for Surface Diffraction	219
6.3.1	Approaching the Classical Limit	225
6.3.2	Selective Adsorption Resonances	231
6.4	Classical Stochastic Theory	238
6.4.1	Elastic Scattering	238
6.4.2	Inelastic Scattering	240
	References	247
7	Scattering from Surface Defects and Activated Diffusion	249
7.1	Introduction	249
7.2	Wave-Packet Calculations and Quantum Trajectories	249
7.3	Vortical Dynamics	258
7.4	Activated Surface Diffusion	260
	References	268
8	Many-Body Systems and Quantum Hydrodynamics	271
8.1	Introduction	271
8.2	The Born-Oppenheimer Approximation	274
8.3	Quantum Hydrodynamics and DFT	276
8.3.1	Time-Independent DFT	276
8.3.2	Time-Dependent DFT	278
8.3.3	Quantum Fluid Dynamic DFT	280
8.4	Quantum Equations of Change	283
8.5	Quantum Flux Conservation	285
8.5.1	Bohmian Probability Tubes	288
8.5.2	Connecting Sections of Initial and Final States	290
8.5.3	A Bohm-Born Rule	291
8.5.4	Quantum Flux Conservation in Tunneling Processes	291
8.5.5	Quantum Flux Conservation in Grating Diffraction	294
	References	297
	Epilogue	305
	Appendix Computing Bohmian Trajectories from the Wave Function:	
	The Analytic Approach	309
A.1	Introduction	309
A.2	Heller's Semiclassical Wave Packets	310
A.2.1	Wave-Packet Evolution	310
A.2.2	Scattering Plane Waves	313
A.2.3	Dissipative Evolution	317
A.3	Simple Spectral Methods	320
A.4	Grid Methods	323
A.4.1	Time-Evolution	324

A.4.2	Spatial Propagation	325
A.4.3	Bohmian Trajectories	327
References		328
Index		331