

Contents

Preface	v
Outline of Boxes	xv
Historical Comments with Portraits	xvii
Sources for Portraits of Physicists	xix
Permissions for Use of Figures	xxi
 1 Introduction to Quantum Trajectories	 1
1.1 Dynamics with Quantum Trajectories	1
1.2 Routes to Quantum Trajectories	7
1.3 The Quantum Trajectory Method	11
1.4 Derivative Evaluation on Unstructured Grids	14
1.5 Applications of the Quantum Trajectory Method	17
1.6 Beyond Bohm Trajectories: Adaptive Methods	18
1.7 Approximations to the Quantum Force	21
1.8 Propagation of Derivatives Along Quantum Trajectories	22
1.9 Trajectories in Phase Space	25
1.10 Mixed Quantum–Classical Dynamics	27
1.11 Additional Topics in Quantum Hydrodynamics	30
1.12 Quantum Trajectories for Stationary States	32
1.13 Coping with Problems	33
1.14 Topics Not Covered	36
1.15 Reading Guide	37
 2 The Bohmian Route to the Hydrodynamic Equations	 40
2.1 Introduction	40
2.2 The Madelung–Bohm Derivation of the Hydrodynamic Equations	 42
2.3 The Classical Hamilton–Jacobi Equation	48
2.4 The Field Equations of Classical Dynamics	52
2.5 The Quantum Potential	53
2.6 The Quantum Hamilton–Jacobi Equation	56
2.7 Pilot Waves, Hidden Variables, and Bohr	59

3	The Phase Space Route to the Hydrodynamic Equations	62
3.1	Introduction	62
3.2	Classical Trajectories and Distribution Functions in Phase Space	65
3.3	The Wigner Function	68
3.4	Moments of the Wigner Function	74
3.5	Equations of Motion for the Moments	77
3.6	Moment Analysis for Classical Phase Space Distributions	80
3.7	Time Evolution of Classical and Quantum Moments	83
3.8	Comparison Between Liouville and Hydrodynamic Phase Spaces	85
3.9	Discussion	86
4	The Dynamics and Properties of Quantum Trajectories	89
4.1	Introduction	89
4.2	Equations of Motion for the Quantum Trajectories	90
4.3	Wave Function Synthesis Along a Quantum Trajectory	94
4.4	Bohm Trajectory Integral Versus Feynman Path Integral	97
4.5	Wave Function Propagation and the Jacobian	99
4.6	The Initial Value Representation for Quantum Trajectories	101
4.7	The Trajectory Noncrossing Rules	104
4.8	Dynamics of Quantum Trajectories Near Wave Function Nodes	104
4.9	Chaotic Quantum Trajectories	109
4.10	Examples of Chaotic Quantum Trajectories	112
4.11	Chaos and the Role of Nodes in the Wave Function	117
4.12	Why Weren't Quantum Trajectories Computed 50 Years Ago?	119
5	Function and Derivative Approximation on Unstructured Grids	123
5.1	Introduction	123
5.2	Least Squares Fitting Algorithms	127
5.3	Dynamic Least Squares	132
5.4	Fitting with Distributed Approximating Functionals	135
5.5	Derivative Computation via Tessellation and Fitting	138
5.6	Finite Element Method for Derivative Computation	141
5.7	Summary	144
6	Applications of the Quantum Trajectory Method	148
	<i>Corey J. Trahan</i>	
6.1	Introduction	148
6.2	The Free Wave Packet	150
6.3	The Anisotropic Harmonic Oscillator	153
6.4	The Downhill Ramp Potential	156
6.5	Scattering from the Eckart Barrier	161
6.6	Discussion	163

7 Adaptive Methods for Trajectory Dynamics	166
<i>Corey J. Trahan</i>	
7.1 Introduction	166
7.2 Hydrodynamic Equations and Adaptive Grids	167
7.3 Grid Adaptation with the ALE Method	169
7.4 Grid Adaptation Using the Equidistribution Principle	172
7.5 Adaptive Smoothing of the Quantum Force	177
7.6 Adaptive Dynamics with Hybrid Algorithms	182
7.7 Conclusions	187
8 Quantum Trajectories for Multidimensional Dynamics	190
8.1 Introduction	190
8.2 Description of the Model for Decoherence	191
8.3 Quantum Trajectory Results for the Decoherence Model	194
8.4 Quantum Trajectory Results for the Decay of a Metastable State	199
8.5 Quantum Trajectory equations for Electronic Nonadiabatic Dynamics	203
8.6 Description of the Model for Electronic Nonadiabatic Dynamics	211
8.7 Nonadiabatic Dynamics From Quantum Trajectory Propagation	214
8.8 Conclusions	215
9 Approximations to the Quantum Force	218
9.1 Introduction	218
9.2 Statistical Approach for Fitting the Density to Gaussians	219
9.3 Determination of Parameters: Expectation-Maximization	220
9.4 Computational Results: Ground Vibrational State of Methyl Iodide	222
9.5 Fitting the Density Using Least Squares	225
9.6 Global Fit to the Log Derivative of the Density	227
9.7 Local Fit to the Log Derivative of the Density	230
9.8 Conclusions	233
10 Derivative Propagation Along Quantum Trajectories	235
10.1 Introduction	235
10.2 Review of the Hydrodynamic Equations	236
10.3 The DPM Derivative Hierarchy	237
10.4 Implementation of the DPM	240
10.5 Two DPM Examples	241
10.6 Multidimensional Extension of the DPM	244
10.7 Propagation of the Trajectory Stability Matrix	246
10.8 Application of the Trajectory Stability Method	249
10.9 Comments and Comparisons	250

11 Quantum Trajectories in Phase Space	254
11.1 Introduction	254
11.2 The Liouville, Langevin, and Kramers Equations	255
11.3 The Wigner and Husimi Equations	260
11.4 The Caldeira–Leggett Equation	266
11.5 Phase Space Evolution with Entangled Trajectories	270
11.6 Phase Space Evolution Using the Derivative Propagation Method	271
11.7 Equations of Motion for Lagrangian Trajectories	273
11.8 Examples of Quantum Phase Space Evolution	275
11.9 Momentum Moments for Dissipative Dynamics	285
11.10 Hydrodynamic Equations for Density Matrix Evolution	288
11.11 Examples of Density Matrix Evolution with Trajectories	292
11.12 Summary	295
12 Mixed Quantum–Classical Dynamics	300
12.1 Introduction	300
12.2 The Ehrenfest Mean Field Approximation	301
12.3 Hybrid Hydrodynamical–Liouville Phase Space Method	302
12.4 Example of Mixed Quantum–Classical Dynamics	307
12.5 The Mixed Quantum–Classical Bohmian Method (MQCB)	308
12.6 Examples of the MQCB Method	312
12.7 Backreaction Through the Bohmian Particle	316
12.8 Discussion	318
13 Topics in Quantum Hydrodynamics: The Stress Tensor and Vorticity	322
13.1 Introduction	322
13.2 Stress in the One-Dimensional Quantum Fluid	323
13.3 Quantum Navier–Stokes Equation and the Stress Tensor	328
13.4 A Stress Tensor Example	329
13.5 Vortices in Quantum Dynamics	334
13.6 Examples of Vortices in Quantum Dynamics	336
13.7 Features of Dynamical Tunneling	343
13.8 Vortices and Dynamical Tunneling in the Water Molecule	344
13.9 Summary	350
14 Quantum Trajectories for Stationary States	354
14.1 Introduction	354
14.2 Stationary Bound States and Bohmian Mechanics	355
14.3 The Quantum Stationary Hamilton–Jacobi Equation: QSHJE	356
14.4 Floydian Trajectories and Microstates	357
14.5 The Equivalence Principle and Quantum Geometry	363
14.6 Summary	366

15 Challenges and Opportunities	369
15.1 Introduction	369
15.2 Coping with the Spatial Derivative Problem	371
15.3 Coping with the Node Problem	372
15.4 Decomposition of Wave Function into Counterpropagating Waves	378
15.5 Applications of the Covering Function Method	382
15.6 Quantum Trajectories and the Future	387
Appendix 1: Atomic Units	389
Appendix 2: Example QTM Program	390
Index	395