

Contents

<i>Foreword</i>	page x
<i>Contributors</i>	xiii
<i>Preface</i>	xvii
Part I Introduction	
1 Quantum biology: introduction	3
GRAHAM R. FLEMING AND GREGORY D. SCHOLES	
1.1 Introduction	3
1.2 Excited states in biology	4
1.3 Light particles and tunnelling	7
1.4 Radical pairs	8
1.5 Questions for the present	9
1.6 Some wide-reaching questions	12
2 Open quantum system approaches to biological systems	14
ALIREZA SHABANI, MASOUD MOHSENI, SEOGJOO JANG, AKIHITO ISHIZAKI, MARTIN PLENIO, PATRICK REBENTROST, ALAN ASPURU-GUZI, JIANSHU CAO, SETH LLOYD AND ROBERT SILBEY	
2.1 Quantum mechanics concepts and notations	15
2.2 Open quantum systems: dynamical map approach	17
2.3 Open quantum systems: master equation approach	21
2.4 Formally exact QME	22
2.5 QME in the weak system-bath coupling limit	24
2.6 QME for weak coupling to a Markovian bath	26
2.7 QMEs beyond weak and Markovian limits	28
2.8 Second-order cumulant time-non-local equation and its hierarchical representation	33
2.9 A post-perturbative time convolution QME	35
2.10 QME in the polaron picture	38

2.11	Path integral techniques	44
2.12	DMRG based approaches	47
3	Generalized Förster resonance energy transfer	53
	SEOGJOO JANG, HODA HOSSEIN-NEJAD AND GREGORY D. SCHOLES	
3.1	Introduction	53
3.2	Förster's rate expression: a complete derivation	56
3.3	Transition density cube method	62
3.4	Generalized Förster theories	65
3.5	Important computational issues in an actual application	72
3.6	Applications of MC-FRET	77
3.7	Summary	81
4	Principles of multi-dimensional electronic spectroscopy	82
	TOMÁŠ MANČAL	
4.1	Photo-induced dynamics of molecular systems	82
4.2	Non-linear response of multi-state systems	89
4.3	Cumulant expansion of a non-linear response	99
4.4	Selected non-linear spectroscopic methods	106
4.5	Conclusions	119
Part II Quantum effects in bacterial photosynthetic energy transfer		
5	Structure, function, and quantum dynamics of pigment-protein complexes	123
	IOAN KOŠZTIN AND KLAUS SCHULTEN	
5.1	Introduction	123
5.2	Light-harvesting complexes from purple bacteria: structure, function and quantum dynamics	125
5.3	Optical transitions in pigment-protein complexes	131
5.4	Electron transfer in pigment-protein complexes	140
6	Direct observation of quantum coherence	144
	GREGORY S. ENGEL	
6.1	Detecting quantum coherence	144
6.2	Observation of quantum coherence using 2D electronic spectroscopy	147
6.3	Identifying and characterizing quantum coherence signals	151
6.4	Quantum coherence in reaction centres using two colour electronic coherence photon echo spectroscopy	155
6.5	Observing quantum coherences at physiological temperatures	156
6.6	Outlook for future measurements of coherence	157

7	Environment-assisted quantum transport	159
	MASOUD MOHSENI, ALÁN ASPURU-GUZZI, PATRICK REBENTROST, ALIREZA SHABANI, SETH LLOYD, SUSANA F. HUELGA AND MARTIN B. PLENIO	
7.1	Introduction	159
7.2	Master equations for quantum transport	161
7.3	Quantum transport in a two-chromophore system	162
7.4	The principles of noise-assisted quantum transport	164
7.5	Quantum transport in the Fenna–Matthews–Olson protein complex	167
7.6	Optimality and robustness of quantum transport	170
7.7	Conclusion	175
Part III Quantum effects in higher organisms and applications		
8	Excitation energy transfer and energy conversion in photosynthesis	179
	ELISABET ROMERO, VLADIMIR I. NOVODEREZHKIN AND RIENK VAN GRONDELLE	
8.1	Photosynthesis	179
8.2	Photosynthetic energy conversion: charge separation	180
8.3	Light-harvesting	190
9	Electron transfer in proteins	198
	SPIROS S. SKOURTIS	
9.1	Introduction	198
9.2	The rate for a single-step electron transfer reaction mediated by elastic through-bridge tunnelling	201
9.3	Dependence of tunnelling on protein structure: tunnelling pathways and their interferences	205
9.4	Tunnelling matrix element fluctuations in deep-tunnelling ET reactions	208
9.5	Vibrational quantum effects and inelastic tunnelling	211
9.6	Biological ET chains with tunnelling and hopping steps through the protein medium	214
9.7	Conclusions	216
9.8	Acknowledgements	217
10	A chemical compass for bird navigation	218
	ILIA A. SOLOV'YOV, THORSTEN RITZ, KLAUS SCHULTEN AND PETER J. HORE	
10.1	Introduction	218
10.2	Theoretical basis for a chemical compass	221

10.3	In vitro magnetic field effects on radical pair reactions	227
10.4	Evidence for a radical pair mechanism in birds	232
10.5	Conclusion	236
11	Quantum biology of retinal	237
	KLAUS SCHULTEN AND SHIGEHICO HAYASHI	
11.1	Introduction	237
11.2	Retinal in rhodopsin and bacteriorhodopsin	238
11.3	Quantum physics of excited state dynamics	242
11.4	Regulation of photochemical processes for biological function	245
11.5	Potential energy crossing and conical intersection	246
11.6	Electronic structure of protonated Schiff base retinal	252
11.7	Mechanism of spectral tuning in rhodopsins	255
11.8	Photoisomerization of retinal in rhodopsins	257
11.9	Summary and outlook	262
11.10	Acknowledgement	263
12	Quantum vibrational effects on sense of smell	264
	A.M. STONEHAM, L. TURIN, J.C. BROOKES AND A.P. HORSFIELD	
12.1	Phonon assisted tunnelling in olfaction	264
12.2	Important processes and timescales	267
12.3	Quantum rate equations	271
12.4	Putting in numbers	272
12.5	Can we make predictions?	275
12.6	Extensions of the theory for enantiomers	275
13	A perspective on possible manifestations of entanglement in biological systems	277
	HANS J. BRIEGEL AND SANDU POPESCU	
13.1	Introduction	277
13.2	Entanglement	278
13.3	Non-local correlations	281
13.4	Entanglement in biology	289
13.5	Open driven systems and entanglement	292
13.6	Conclusions	310
14	Design and applications of bio-inspired quantum materials	311
	MOHAN SAROVAR, DÖRTHE M. EISELE AND K. BIRGITTA WHALEY	
14.1	Potential applications of bio-inspired quantum materials	311
14.2	Progress in designing biomimetic quantum materials	315

15	Coherent excitons in carbon nanotubes	335
	LEONAS VALKUNAS AND DARIUS ABRAMAVICIUS	
15.1	Structure	335
15.2	Electronic properties in 1D systems	335
15.3	Exciton-exciton interactions	339
15.4	Non-linear optical response of excitons	343
15.5	Simulations of intensity-dependent 3PEPS	345
15.6	Discussion and conclusions	347
15.7	Acknowledgement	349
	References	350
	Index	396