## **Contents**

1	Intr	roduction 1				
1.1 Quantum practicality				1		
	1.2	2 Models of quantum simulation				
	1.3	Proble	ems in quantum chemistry	6		
		1.3.1	Electronic structure problem	6		
		1.3.2	Quantum dynamics	11		
		1.3.3	Computational complexity	13		
	1.4	Quant	rum computing basics	13		
		1.4.1	Quantum building blocks	13		
		1.4.2	Encoding fermionic problems on quantum computers	15		
1.5 Quantum algorithms for quantum			rum algorithms for quantum chemistry	16		
		1.5.1	Quantum phase estimation	17		
		1.5.2	Variational quantum eigensolver	18		
		1.5.3	Quantum imaginary time evolution	20		
	1.6	Outlin	e of the dissertation	22		
2	Λ -	14i	former another Verilar already for the -t			
4	<b>A</b> 1	munnre	ference quantum Krylov algorithm for strongly-			
	corr	elated	electrons	23		

	2.1	Metho	ods	28						
		2.1.1	Basis in MRSQK	28						
		2.1.2	State Preparation	33						
		2.1.3	Quantum Circuits for Measuring Matrix Elements	34						
		2.1.4	Cost Estimation	37						
	2.2	Comp	utational Details	40						
	2.3	Results and Discussion								
	2.4	Summary								
	2.5	Appen	ıdix	49						
		2.5.1	Trotterization errors and term ordering	49						
		2.5.2	Comments	56						
	2.6	Comp	uting electronic excited states via multireference quan-							
		tum K	rylov method	57						
		2.6.1	state-specific approach	57						
		2.6.2	state-averaged approach with dynamic weights	59						
3	Leveraging small scale quantum computers with unitarily down-									
	fold	ed Han	niltonians	64						
	3.1	Metho	ods	69						
		3.1.1	Unitary Hamiltonian downfolding via the DSRG	69						
		3.1.2	Hybrid quantum-classical DSRG downfolding	73						
	3.2	2 Calibration		80						
		3.2.1	Noiseless simulations	80						
		3.2.2	Sensitivity to noise	83						
	3.3	Result	s and Discussion	86						

		3.3.1	Dissociation curve of the nitrogen molecule 87	7	
		3.3.2	Singlet-triplet gaps of <i>para</i> -benzyne 90	0	
		3.3.3	Hardware implementation	3	
	3.4	Summ	ary 10	1	
	3.5	Appendix			
		3.5.1	Symmetry-preserving ansatz for two-configuration		
			wave functions	4	
		3.5.2	Comparing QDSRG with double unitary coupled cluster		
			approach	8	
4 Simulating conical intersections on quantum computers with un					
4	Sim	ulating	conical intersections on quantum computers with uni-		
4			conical intersections on quantum computers with uni- nfolded Hamiltonians	0	
4		y dowi	•		
4	taril	y down	nfolded Hamiltonians 110	3	
4	taril	y down	nfolded Hamiltonians  110  ds	3	
4	taril	y down Metho	nfolded Hamiltonians  110  ds	3 3 5	
4	taril	Metho 4.1.1 4.1.2 4.1.3	Infolded Hamiltonians  ods	3 3 5 6	
4	taril	Metho 4.1.1 4.1.2 4.1.3 Comp	Infolded Hamiltonians  ods	3 3 5 6 7	
4	<b>taril</b> 4.1	Methodology 4.1.1 4.1.2 4.1.3 Compo	Infolded Hamiltonians       110         Inds       110 <th>3 3 5 6 7 8</th>	3 3 5 6 7 8	