

Contents

	Preface	<i>IX</i>
1	A First Monte Carlo Example	<i>1</i>
1.1	Energy of Interacting Classical Gas	<i>1</i>
1.1.1	Classical Many-Particle Statistics and Some Thermodynamics	<i>2</i>
1.1.2	How to Sample the Particle Density?	<i>18</i>
2	Variational Quantum Monte Carlo for a One-Electron System	<i>23</i>
3	Two Electrons with Two Adiabatically Decoupled Nuclei: Hydrogen Molecule	<i>39</i>
3.1	Theoretical Description of the System	<i>39</i>
3.2	Numerical Results of Moderate Accuracy	<i>42</i>
3.3	Controlling the Accuracy	<i>46</i>
3.4	Details of Numerical Program	<i>53</i>
4	Three Electrons: Lithium Atom	<i>61</i>
4.1	More Electrons, More Problems: Particle and Spin Symmetry	<i>63</i>
4.1.1	Antisymmetry and Decomposition of the Many-Body Wave Function	<i>63</i>
4.1.2	Three-Electron Wave Function	<i>65</i>
4.1.3	General Wave Function	<i>67</i>
4.1.4	Relaxing Symmetry of Total Spin	<i>70</i>
4.2	Electron Orbitals for the Slater Determinant	<i>71</i>
4.3	Slater Determinants: Evaluation and Update	<i>76</i>
4.4	Some Important Observables in Atoms?	<i>82</i>
4.4.1	The Module “observables”	<i>87</i>
4.5	Statistical Accuracy	<i>91</i>
4.6	Ground State Results	<i>93</i>
4.6.1	Results for Lithium Atom	<i>93</i>
4.6.2	Code of Main Program, Modules of Variables, of Statistic, of Jastrow Factor, and of Output	<i>103</i>
4.7	Optimization?	<i>115</i>
5	Many-Electron Confined Systems	<i>121</i>
5.1	Model Systems with Few Electrons	<i>121</i>

5.2	Orthorhombic Quantum Dot	122
5.2.1	Confined Single-Particle Wave Functions	122
5.2.2	Details of Program	123
5.2.3	Energy and Radial Density	125
5.2.4	Pair-Correlation Function	131
5.2.5	Program of the Pair-Correlation Function	134
5.3	Spherical Quantum Dot	136
5.3.1	Fundamentals of DFT	137
5.3.2	DFT Calculation of the Jellium Cluster: Methodology	138
5.3.3	QMC Calculation of the Jellium Cluster: Methodology	140
5.3.4	QMC Code for the Calculation of Jellium Clusters	141
5.3.5	Comparison between DFT and QMC Calculations of Jellium Clusters	142
6	Many-Electron Atomic Aggregates: Lithium Cluster	147
6.1	Clusters and Nanophysics	147
6.2	Cubic BCC Arrangement of Lithium Atoms	150
6.2.1	Structure of the Main Program	150
6.2.2	Single-Electron Wave Functions and Structure of the Determinant	150
6.2.3	Geometric Setting of the Cluster	153
6.2.4	Changes in the Program	156
6.3	The Cluster: Intermediate between Atom and Solid	163
6.3.1	$1 \times 1 \times 1$ Cluster: Li_2	164
6.3.2	$2 \times 2 \times 2$ Cluster	167
6.3.3	$3 \times 3 \times 3$ Cluster	172
6.3.4	$4 \times 4 \times 4$ Cluster	174
6.3.5	Cluster Size	178
7	Infinite Number of Electrons: Lithium Solid	181
7.1	Infinite Lattice	183
7.1.1	The Lattices	183
7.1.2	Structure of the Electrostatic Potential	186
7.1.3	Ewald Summation and Tabulation	191
7.1.4	Finite-Size Effects	204
7.2	Wave Function	208
7.2.1	Linear Combination of Atomic Orbitals	208
7.2.2	Plane Waves	210
7.3	Jastrow Factor	212
7.3.1	Standard Choice	213
7.3.2	Principal Ideas and Extensions	215
7.4	Results for the $3 \times 3 \times 3$ and $4 \times 4 \times 4$ Superlattice Solid	216
8	Diffusion Quantum Monte Carlo (DQMC)	223
8.1	Towards a First DQMC Program	224
8.1.1	Relating Schrödinger Equation to Diffusion	224
8.1.2	Generate Gaussian Random Numbers	228

8.1.3	Application	229
8.1.3.1	Harmonic Oscillator	229
8.2	Conclusion	235
9	Epilogue	237
	Appendix	239
A.1	The Interacting Classical Gas: High Temperature Asymptotics	239
A.2	Pseudorandom Number Generators	241
A.3	Some Generalization of the Jastrow Factor	247
A.4	Series Expansion	249
A.5	Wave Function Symmetry and Spin	257
A.5.1	Four Electrons	257
A.6	Infinite Lattice: Ewald Summation	259
A.7	Lattice Sums: Calculation	263
	References	269
	Index	273

