

Contents

1	Introduction	7
1.1	Discovery of quasi-periodic materials	7
1.2	What is the quasi-periodicity?	8
1.3	Previous studies	13
1.3.1	Peculiar electronic states due to quasi-periodicity	13
1.3.2	Effect of electron correlations	19
1.4	Aim of this study	20
1.5	Outline of this thesis	22
2	Models and methods	23
2.1	Construction of quasi-periodic lattices	23
2.1.1	One-dimensional Fibonacci lattice	24
2.1.2	Two-dimensional Penrose lattice	24
2.1.3	Three-dimensional Penrose lattice	28
2.2	Models	29
2.2.1	Ising model	29
2.2.2	Falicov-Kimball model	30
2.3	Monte Carlo method	31
2.3.1	Importance sampling	31
2.3.2	Replica-exchange Monte Carlo method	33
3	Results for the Ising model	35
3.1	Antiferromagnetic order without frustration	35
3.1.1	Phase transition	36
3.1.2	Correlation function	37
3.2	Effect of frustration	46
4	Results for the Falicov-Kimball model	51
4.1	Noninteracting case	51
4.2	Antiferromagnetic order at half-filling	56
4.3	Carrier doping	60
4.3.1	Filling plateau—peculiar Mott insulator	60
4.3.2	Real-space distribution of electrons in the filling plateau	65

4.3.3 Occupation rules in the peculiar Mott insulator	68
5 Summary	72