

Gutzwiller study for phase diagram of extended Hubbard models with fixed boson densities

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We studied the phase diagram of extended Bose–Hubbard models with nearest-neighbor interaction on bipartite lattices in a canonical ensemble by using the Gutzwiller variational wave function and the linear programming method under the condition of fixed boson densities. Contrary to the hard-core model, the soft-core model at half filling has a possible SS phase between the solid and SF phases and all phase transitions are continuous. We also found that the phase diagram of the soft-core model strongly depends on its transfer integral t . For small t , the shape of the SF region is similar to that of the hard-core model with particle-hole symmetry and the SS phase does not appear because of the phase separation above half filling. In contrast, for large t , the SS phase appears even above half filling. The phase diagram becomes simplified for large t , where there is only a continuous SF–SS phase transition and the critical value of t at the phase boundary is a smooth decreasing function of boson density N .

Finally, we also found that the density difference between nearest-neighbor sites δn , which shows the density wave order of the SS phase, strongly depends on the boson density N . In particular, for small t , the difference δn is a discontinuous function of the nearest-neighbor interaction V and is larger for smaller (larger) N for small (large) V .