Quantum Phase Transitions in Correlated Systems

(Ph.D. thesis points)

Ákos Rapp
Budapest University of Technology and Economics
Department of Theoretical Physics

Supervisor:
Prof. Gergely Zaránd

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Background

Numerous materials and physical systems exhibiting strong correlations show anomalous behavior at low temperatures. In many cases, the origin of these anomalies is a second order quantum phase transition at zero temperature. The complete understanding of the quantum critical behavior emerging from this transition represents one of the most challenging problems in modern condensed matter physics.

Quantum phase transitions can be investigated efficiently in one dimension, since models in low dimensions can be analyzed using powerful mathematical tools. The ground state dynamics of one-dimensional spin models has been studied extensively, and in many cases, finite temperature static properties have also been discussed. On the other hand, the finite temperature dynamical behavior of gapped one-dimensional models is much less understood. The aim of part of the present work was to understand dynamical properties of gapped systems in one dimension, with a particular emphasis on the role of internal degrees of freedom.

The other focus of this work was the quantum phase transitions in ultracold atomic systems. Recently it became possible to trap both bosonic and fermionic atoms in optical lattices in ultracold environments, furthermore, one can also create mixtures with both particle species. The hyperfine quantum numbers of these atoms offer a large number of variational possibilities for experiments, and provide new fields for theoretical investigations. In the experiments with ultracold atomic gases, it is possible to realize systems of locally interacting particles on a lattice, where the number of “spin components” is not limited to two. A generalization of the Hubbard model with multiple spin components provides a good description of such systems. Although the two-component Hubbard model has been the subject of intense research, the ground states of its general, multicomponent versions have not been investigated in great detail.

Goals

In the first part of the thesis, I study finite temperature dynamical correlations in the $Q = 3$ state quantum Potts model in one dimension. The quantum Potts model exhibits a phase transition at zero temperature, which appears between a ferromagnetic and a quantum paramagnetic ground state. The discussions of the quantum critical regime and the low temperature gapped phases need different approaches. In the quantum critical region, the dynamics is determined by scaling exponents of the quantum critical point. I derive the dynamical susceptibility in this region using the tools of conformal field theory and a Fourier transformation. On the other hand, in the gapped phases, scattering of the quasiparticles with internal quantum numbers also leads to non-trivial dynamics. Although I can use a semiclassical approximation to calculate the correlation functions, first I have to understand the quantum mechanics of two-particle collisions. I also discuss how the semiclassical method applied to the Potts model can be generalized to other gapped one-dimensional models.

In the second part of the thesis, I discuss the ground state properties of the attractive three-component Hubbard model in infinite dimensions within a Gutzwiller calculation. Similar to the two-component case, there is a transition between two limiting regimes, which are dominated by the kinetic and interaction energies, respectively. I study this transition which turns out to be a phase transition. I discuss the weakly and strongly interacting limits to find the appropriate Gutzwiller ansatz. The calculation of Gutzwiller expectation values is a complicated many-body problem: I construct a functional integral formalism to evaluate these expectation values exactly in infinite dimensions. I interpret the results of the infinite-dimensional Gutzwiller calculations for possible experimental realizations.

New scientific results

I. Using the critical exponents of the $Q = 3$ state classical Potts model in $d = 2$ dimensions, I constructed the correlation function of the $d = 1$ dimensional quantum Potts model at the critical point, $g = g_c$ and $T = 0$. I applied a conformal mapping to obtain the imaginary time dynamical correlation function at finite temperature. Based on the analytic properties of this expression, I performed a Fourier transformation and analytic continuation on the complex frequency plain to obtain the dynamical susceptibility in the quantum critical region, at $g = g_c$ and $T > 0$ [1].

II. I provided two arguments that the small - momentum limit of the two-particle scattering matrix in the gapped phases of the $Q = 3$ quantum Potts model is of purely exchange type. Based on this structure of the $\mathcal{S}$-matrix, I calculated the dynamical correlation functions analytically in the semiclassical limit $T \ll \Delta$. The relaxation function of correlations showed universal diffusive behavior both on the ferromagnetic and on the paramagnetic sides. I reproduced the semiclassical results for the Ising model in a transverse magnetic field in a simple way, in the limit $Q = 2$ [1].

III. Using the semiclassical method, I calculated the $n^z - n^z$ dynamical correlation function of the O(3) quantum rotor model, which is related to the inelastic neutron-scattering lineshape of the S=1 antiferromagnetic Heisenberg chain at wave number $q \approx \pi$. I generalized the method to $O(N)$ quantum rotor models and also showed that the same relaxation function describes the correlations in the sine-Gordon model in the semiclassical limit. I thus found that the relaxation function derived analytically for the quantum Potts model applies to a variety of systems. I found for long timescales an exponential decay of correlations for the parameter $Q = 2$ in the relaxation function, while I found diffusive decay for $Q > 2$ [4].

IV. Based on symmetry arguments, I showed that there is a phase transition in the SU(3) attractive Hubbard model at zero temperature as a function of the interaction strength. Analyzing the strong coupling limit, I found that the most important correlations can be captured in a Gutzwiller type wave function (in the limit of $d = \infty$ dimensions) to describe the color superfluid – trionic phase transition. I constructed a mapping to an effective field theory to calculate the Gutzwiller expectation values. This functional integral formalism could be generalized to other Gutzwiller calculations as well [2, 3].

V. Based on the cavity method of dynamical mean field theory, I solved the effective field theory in the $d = \infty$ dimensional limit. I evaluated the Gutzwiller expectation values exactly in infinite dimensions in terms of the proper self-energy matrix of the effective field theory. I solved the selfconsistency equations for the self-energy matrix numerically. The results of the Gutzwiller calculation showed that a second order quantum phase transition appears between the color superfluid and the trionic phase, away from half filling. I determined the critical values of the interaction strength as a function of the filling factor. I also observed that the spontaneous breaking of SU(3) symmetry by the superfluid order is accompanied by "ferromagnetism" [2, 3].

VI. I performed modified Gutzwiller calculations using a semicircular single-particle density of states or with anisotropic interactions between the different hyperfine components that explicitly break the SU(3) symmetry. I observed that there are no qualitative differences compared to the case with SU(3) symmetry and a Gaussian density of states, and that the continuous phase transition seems to persist. These results indicated that the phase transition found is robust and could be observed experimentally [3].

References

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