Scientific report

December 2014 – December 2015

Thermodynamic Properties and Correlation Functions of Low-Dimensional Ultracold Gases

Team

Ovidiu I. Patu CS III (Principal Investigator), Cecil Pompiliu Grunfeld CS I

Results

ISI Articles

 [P1] Ovidiu I. Patu, <u>Correlation functions and momentum distribution of one-dimensional hard-core anyons</u> <u>in optical lattices</u>, J. Stat. Mech. P01004 (2015) [Impact factor (2014) 2.404, Top 25% Mathematical Physics] [arXiv:1409.2321] (submitted in 2014)

[PK2] Ovidiu I. Patu and Andreas Klumper, <u>Thermodynamics, density profiles and correlation functions of</u> <u>the inhomogeneous one-dimensional spinor Bose gas</u>, Phys. Rev. A, **92** 043631 (2015), [Impact factor (2014) 2.808, Top 25% Optics]

Articles in preparation

[PK3] Ovidiu I. Patu and Andreas Klumper, *Thermodynamics, contact and density profiles of the repulsive Gaudin-Yang model*

[PK4] Ovidiu I. Patu and Andreas Klumper, *Thermodynamics and local correlation functions of the Bose-Fermi mixture*

Scientific activities

Local correlation functions and contact of the repulsive Gaudin-Yang model. The Gaudin-Yang model, also known as the two-component Fermi gas (2CFG), was the first multi-component model solved by the Nested Bethe Ansatz in the late 1960's. The thermodynamics of this model in the framework of the Thermodynamic Bethe Anstaz (TBA) was discovered by Takahashi and Lai in the 70's but the complexity of the TBA equations (an infinite system of coupled non-linear integral equations) meant that theoretical and numerical investigations of the thermodynamics were confined to the strong-coupling and low-temperature regime. In the previous stage of the project, using the lattice embedding of the 2CFG in the q=3 Perk-Schultz spin chain and the quantum transfer matrix method we have derived an efficient thermodynamic description for the repulsive Gaudin-Yang model which is valid for all values of the relevant parameters: temperature, coupling strength, chemical potential and magnetic field. Our result obtained for the grandcanonical potential is extremely simple :

$$\phi(\mu, H, T) = \frac{-T}{2\pi} \int \ln(1 + a_1(k)) + \ln(1 + a_2(k)) dk$$

where μ , H, T is the chemical potential, magnetic field and temperature and the auxiliary functions $a_{1,2}$ satisfy the system of equations

$$\ln a_1(k) = -\frac{(k^2 - \mu - H)}{T} + \int_{\mathbb{R}^{-i\epsilon}} K_2(k - k') \ln(1 + a_2(k')) dk' \quad K_2(k) = \frac{1}{k(k - ic)}$$

$$\ln a_{2}(k) = -\frac{(k^{2} - \mu + H)}{T} + \int_{\mathbb{R} + i\epsilon} K_{1}(k - k') \ln(1 + a_{1}(k')) dk' \quad K_{1}(k) = \frac{1}{k(k + ic)}$$

This system of two non-linear integral equations (NLIEs) can be easily implemented numerically by moving the contours of integration in the upper and lower half-plane and evaluating the convolutions using the Fast Fourier Transform (FFT) and the convolution theorem.

In addition to deriving the thermodynamic properties and density profiles of the model (which were obtained in the previous stage of the project) the NLIEs can also be used to compute the local correlation function of opposite spins and the contact. S. Tan discovered that the momentum distribution of 3D fermions with short-range interactions falls like C/k^4 where C is a quantity called contact which is the same for both species of particles (spin up and down) and is closely related with the local correlation function of opposite spins which quantifies the probability that two particles of opposite spins can be found in the same point in space. The contact also appears in series of thermodynamic universal relations relating the pressure, interaction and trapping energy of which we remember Tan's adiabatic theorem. We have performed an extensive investigation of the contact, local correlation function and interaction energy of the 2CFG as follows:

- At finite temperature we have used the NLIEs (see above) and the Helmann-Feynman theorem from which we derived the local correlation function and contact. Because our result for the thermodynamics was derived in the framework of the grandcanonical ensemble we have used a matrix Newton-Raphson subroutine which scans the chemical potential and magnetic field parameter space and finds the appropriate values for a required value of the density and polarization.
- At T=0 the thermodynamics of the model is characterized by a system of two Fredholm integral equations for the total density and density of spin down particles from which the energy of the groundstate can be determined. The numerical integration of this system was performed using the Nystrom method with the Gauss-Legendre quadrature and the contact was determined from Tan's adiabatic theorem. Similar to the case of finite temperature we have also implemented a matrix Newton-Raphson subroutine in order to obtain the needed density and polarization.
- In the Tonks-Girardeau regime and finite temperature we have also computed the contact from the Fourier transform of the field-field correlator (which is just the momentum distribution). For the impenetrable field-field correlator we have used the Fredholm determinant representation derived by Izergin and Pronko [1] which was numerically implemented using the method suggested by Bornemann [2].

Our results show that the contact is a nonmonotonic function of both the coupling strength and reduced temperature. The importance of this result can be more easily understood if we remember that the contact is the amplitude of the high-momentum tail of the momentum distribution. This means that the nonmonotonicity of the contact results in a change of the shape of the momentum distribution which can be experimentally detected. As a function of the temperature the contact presents a pronounced local minimum in the Tonks-Girardeau regime with the direct result that the momentum distribution becomes narrower as we increase the temperature, behavior which is rather counterintuitive. This is due to the fact that in this case we are dealing with a strongly-interacting system in one dimension which is characterized by spin-charge separation. These results together with the density profiles and thermodynamic quantities are the subject of the forthcoming article [PK3].

Thermodynamics and local correlation functions of the Bose-Fermi mixture The one-dimensional mixture of bosons and fermions interacting via a delta-function potential is also Bethe ansatz solvable. It can be shown that the solutions of the Bethe ansatz equations are all real which means that in principle the application of the TBA method should produce a finite number of equations. However, it seems that the results in the literature do not have the correct behavior in the impenetrable limit (the results should coincide with the one derived for impenetrable fermions). Using the same method employed for the 2CFG and 2CBG we have obtained a system of two NLIEs characterizing the Bose-Fermi mixture which has the correct behavior in the Tonks-Girardeau regime and also reproduces the well-known results in the noninteracting limit. As an additional check we have also shown that the results derived from our NLIEs satisfy with great precision one of Tan's universal thermodynamic identities. We have investigated the thermodynamic properties (densities, specific heat, compressibility, susceptibility) and also the contact and local corelation function which quantifies the probability that a boson and fermion are to be found in the same position in space. Similar to the case of the 2CFG the contact is also a nonmonotonic function of the coupling strength but it also depends strongly on the value of the chemical potential of each species. These results will be presented in the forthcoming article [PK4].

[1] A.G. Izergin and A.G. Pronko, Nucl. Phys. **B** 520, 594 (1998).

[2] F. Bornemann, Math. Comp. 79, 871 (2010).

Principal investigator,

Ovidiu I. Patu