Fractional exclusion statistics in systems with localized states

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Abstract. We develop a model based on the fractional exclusion statistics to describe systems with localized states. The local distribution of the energy levels is captured in the formalism by including the positions in the definition of the species. The particle distributions on the energy axis, as well as in the real space are determined for test-case systems with a peak/dip profile in the local density of states.

1. Introduction
The fundamentals of the fractional exclusion statistics (FES) were introduced by Haldane in his seminal work [1], while the thermodynamical properties of the ideal FES gas were calculated by Wu [2] and Isakov [3]. The formalism was amended recently to include the change of the FES parameters at the change of the particle species [4, 5, 6, 7].

The fractional exclusion statistics is a generalization of the Pauli exclusion principle and in its simplest form represents an interpolation between the Fermi and Bose statistics.

A number of physical systems have been shown to exhibit FES. Amongst them are the quasiparticle excitations at lowest Landau level in the fractional quantum Hall effect, spinon excitations in a spin-$\frac{1}{2}$ quantum antiferomagnet [1, 2], Bose and Fermi systems described in the thermodynamic Bethe ansatz [3, 8, 9, 10], excitations [1] or motifs of spins [11, 12] in spin chains, elementary volumes obtained by coarse-graining in the phase-space of a system [3, 13, 14, 4, 15, 16], etc.

In a more recent study [17], the transition rates in an ideal FES gas were established. The proposed stochastic method generalizes a previous approach for ideal Fermi and Bose gases [18]. The transition rates include the step and the acceptance probabilities. The former component of the transition rate, namely the step probability, is defined in accordance with the generalized exclusion principle. The method can be applied to study non-equilibrium phenomena in interacting Fermi and Bose systems, including disordered, glassy systems, considered from the perspective of ideal FES systems.

Here we extend the FES formalism in order to describe systems with localized states. Concrete applications reside in the area of semiconductor physics (e.g. Coulomb glasses), as well as condensed matter physics (e.g. bosons trapped in optical lattices). In our model the species are organized in order to include the classical degrees of freedom, which are the positions. In section
Figure 1. Partitioning of the real space and the energy axis. The statistical parameters $\alpha_{\xi_i, \eta_j}$ relate the species $(\xi_i)$ and $(\eta_j)$.

2 we present the main features of the formalism and the method of calculation, which includes the specification of the statistical parameters and a discussion of the numerical method employed. Section 3 contains the results obtained in the case of the non-uniform systems considered, which are systems with a peak/dip profile in the local density of states.

2. Formalism and Method

The system consists of a countable set of sites, randomly located at positions $r_I$ in an $s$-dimensional lattice of total volume $\Omega$. Each site may accommodate maximum one particle (fermion). In the absence of particle-particle interaction the energy of the particle on the site is $\epsilon_I$.

We define the species as the elementary volumes in the $(s + 1)$-dimensional position-energy volume, $\Omega \times \epsilon$. The species centered at $r \times \epsilon$ will be denoted by $\delta \Omega_r \times \delta \epsilon$. If the density of sites is $\sigma(r, \epsilon)$, then in the species $\delta \Omega_r \times \delta \epsilon$ we have $G_{\delta \Omega_r \times \delta \epsilon}$ states and $N_{\delta \Omega_r \times \delta \epsilon}$ particles.

For thermodynamic calculations we shall assume that both, $G_{\delta \Omega_r \times \delta \epsilon}$ and $N_{\delta \Omega_r \times \delta \epsilon}$ are much bigger than 1 and the range of $\epsilon$ will be from 0 to $\infty$ in any of the elementary volumes, $\delta \Omega_r$.

The interaction energy between the particles is only position dependent and will be denoted by $V(|r_I - r_J|)$.

The quasiparticle energies will be defined following Ref. [15, 20], as

$$\tilde{\epsilon}_{r_I} = \epsilon_I + \sum_{\tilde{\epsilon}_{r_J} < \tilde{\epsilon}_{r_I}} V(|r_I - r_J|) n_{r_J},$$

where $n_{r_J}$ is the occupation of the site located at $r_J$.

In the quasi-continuous case, assuming that $\tilde{\epsilon}_r(\epsilon) \geq \tilde{\epsilon}_{r'}(\epsilon')$ if $\epsilon \geq \epsilon'$, Eq. (1) becomes

$$\tilde{\epsilon}_r(\epsilon) = \epsilon_I + \int_\Omega d^s r \int_0^\epsilon \sigma(r, \epsilon') V(|r - r'|) n_{r', \epsilon'},$$

where $n_{r', \epsilon}$ is the (average) particle population, defined in any elementary volume as $n_{r', \epsilon} = N_{\delta \Omega_{r', \epsilon}} / G_{\delta \Omega_{r', \epsilon}}$.

The definition (2) leads to the density of sites in the $\Omega \times \tilde{\epsilon}$ space, $\tilde{\sigma}(r, \tilde{\epsilon}) = \sigma(r, \epsilon)(d\tilde{\epsilon}_r(\epsilon)/d\epsilon)^{-1}$, and to the FES parameters [15, 20]:

$$\alpha_{\xi_i, \eta_j} = \delta \Omega_{\xi} \left[ \delta_{ij} \sigma(r_{\xi}, \epsilon_i) + \theta(i - j) \delta \epsilon_i \frac{\partial \sigma(r_{\xi}, \epsilon_i)}{\partial \epsilon_i} \right] \times V(|r_{\xi} - r_{\eta}|).$$

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Figure 2. Particle densities for a peak-peak system (a-b) and for a peak-dip system (c-d). The symbols indicate the index of the species. The insets represent enlarged sections of the main plots.

where the first doublet, \((\xi_i)\), specifies the species in which the number of states changes, whereas the second doublet, \((\eta_j)\), specifies the species in which the number of particle changes; \(\theta(k)\) is the step function, \(\theta(k > 0) = 1\) and \(\theta(k \leq 0) = 0\). Note that the parameters \(\alpha_{\xi_i;\eta_j}\) obey the general rules of Ref. [5] and the ansatz of Ref. [16].

The populations, \(n_{\xi_i}\), are obtained by solving the non-linear system of equations for fermions [16],

\[
0 = \beta(\mu - \xi_i) + \ln \frac{1 - n_{\xi_i}}{n_{\xi_i}} + \sum_{\eta_j} \alpha_{\eta_j;\xi_i} \ln[1 - n_{\eta_j}].
\]  

(4)

Note that the populations \(n_{\xi_i}\) are in general different functions of energy for each site \(\xi\).

The particle density as a function of quasi-particle energy can be expressed as \(\tilde{\rho}(r, \xi, \tilde{\epsilon}) \equiv \tilde{\rho}_{\xi}\) and the spatially integrated density of particles in our discrete approach is \(\tilde{\rho} = \sum_{\xi} \tilde{\rho}_{\xi}\).

The solution of the nonlinear system is found iteratively using gradient descent starting from an initial guess solution. Our implementation used GSL for this purpose.

3. Applications

We consider a one dimensional interacting system of fermions with periodic boundary conditions. The local density of states is assumed to be independent on energy, \(\sigma(r, \epsilon) \equiv \sigma(r)\), and the particle-particle interaction is the screened Coulomb potential,

\[
V(r; \gamma, \lambda) = \kappa \frac{\exp(-r/\lambda)}{r^\gamma},
\]  

(5)

with \(\gamma = 1\) and \(\lambda = 3R_\xi\) being a finite screening length \(-R_\xi\) is the size of the species \(\xi\). In order to remove the singularity at the origin, we take \(V(r) = V(R_0) \equiv V_0\) for \(r < R_0 = R_\xi\). Furthermore we set \(V(R_\xi) = 1\).

For numerical calculations we partition the physical space into \(N_R = 10\) segments (“volumes”) and the energy axis into \(N_E = 50\) segments. This leads to a number of \(N_R \times N_E = 1000\) species. The system contains \(N = N_R E_F \sigma\) particles, where the \(E_F\) is the Fermi energy. In this way we set up the energy scale. The following results are obtained at \(k_B T = 1\).

We analyze two systems with non-uniform density of states. The first system is assumed to have two peaks in the otherwise constant density of states, i.e. \(\sigma_{\xi_1} = 2.0, \sigma_{\xi_2} = 1.5\), while \(\sigma_\xi = 1.0\) for the rest of the species. The results for the particle distributions on the energy axis,
\( \hat{\rho}_\xi \), and in the positions space, \( \hat{\rho}_\xi \) are plotted in Fig. 2(a) and (b), respectively. One can see that the particles tend to accumulate in the two species with higher density of states. The first order neighboring species of both \( \xi_1 \) and \( \xi_2 \) exhibit a drop in the particle density, due to a larger repulsion induced by the particle accumulations at the two sites. Because of this, although the two groups of four species between the peaks have the same density of states (\( \sigma_\xi = 1.0 \)), the particle densities are different.

Next we consider a system with a peak and a dip in the local density of states, i.e. \( \sigma_{\xi_1} = 2.0 \), \( \sigma_{\xi_2} = 0.5 \), while \( \sigma_\xi = 1.0 \) for the rest of the species. The results are plotted in Figs. 2(c) and 2(d). The major difference appears at the species with the lowest density of states. As expected, there is a smaller number of particles in species \( \xi_2 \) than in the rest of the species and because of this the density of particles rises from the species \( \xi_1 + 1 \) to \( \xi_2 - 1 \), as the particles are repelled from the accumulation at \( \xi_1 \).

4. Conclusions
We presented a general method based on the fractional exclusion statistics to extract the equilibrium properties of interacting systems with localized states. The formalism was illustrated on two test-cases of systems with non-uniform density of states – systems with peak/dip profiles in the local density of states.

The method may be extended to a variety of interacting Fermi and Bose systems and may represent an useful tool in calculating the thermodynamical properties of nonuniform interacting particle systems.

Acknowledgments
The work was supported by the Romanian National Authority for Scientific Research projects PN-II-ID-PCE-2011-3-0960 and PN09370102/2009. The travel support from the Romania-JINR Dubna collaboration project Titeica-Markov and project N4063 are gratefully acknowledged.

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