Cyclic *XY* model and exotic statistics in one dimension

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(Received 7 April 1995)

We examine the consequences of the exchange statistics in one-dimensional systems with compact topology. As examples of nontrivial statistical behavior we calculate exactly the partition function and correlators for systems of free q particles on compactified chains. In particular, we consider a spin-1/2 XY chain with periodic boundary conditions that corresponds to the case of $q=-1$. For the case we report a representation of the two-point correlation functions at finite temperature. [S1063-651X(96)50708-7]

PACS number(s): 05.30.−d, 11.30.Pb, 75.10.Jm

In the last decade there has been considerable interest in various deformations of quantum statistics which interpolate between the Bose and Fermi cases. Such deformations can be separated into the deformations of the exchange phase which appears under the permutation of particles (exchange statistics with braiding [1] or without it [2]) and deformations of the Pauli principle (so called exclusion statistics [3]). While the last can be defined in any space dimension the possibility of introducing nontrivial exchange statistics crucially depends on the dimension and the topology.

In one dimension (1D) for particles with a hard-core condition on a finite interval, no real permutation is allowed and, hence, the exchange phase never plays a role. The situation changes if the interval is compactified to a circle with periodic boundary conditions. This leads to a nontrivial loop which provides new possibilities to permute particles via the ''glued'' boundary. Then the effects of exchange statistics immediately exhibit themselves as we demonstrate in this paper. In the framework of our lattice model we calculate exactly the partition function and correlators and, moreover, the result is remarkably simple. The partition functions and correlation functions for a system with such exchange statistics can be written as a double sum of terms indexed by all possible deformations of an exchange factor and all permutation loops in the systems. This suggests that the theory may be reformulated as a theory of loops with weights defined by the deformed exchange factors. Such a theory could then be generalized to higher dimensions.

The point is illustrated by the example of free q fermions, i.e., the particles with deformed exchange statistics defined by the algebra of commutation relations for the creation (annihilation) operators $a_i^\dagger$ (a_i) at the ith site of a cyclic chain with length M. The relations are split into two parts: the first describes the fermionic algebra on each site,

$$a_i^\dagger a_i + a_i a_i^\dagger = 1, \quad a_i^2 = 0, \quad (a_i)^\dagger = a_i^\dagger, \tag{1}$$

and the second gives the exchange statistics with deformation parameter $q=e^{2\pi ir/n}$, $n \geqslant r \geqslant 1$,

$$a_i a_j = -q a_j a_i, \quad a_i^\dagger a_j = -q^{-1} a_j a_i^\dagger, \tag{2}$$

where the ordering $1 \leqslant i < j \leqslant M$ is assumed.

Presently we will consider a gas of free q fermions with the Hamiltonian (qXX model):

$$H = \sum_{i=2}^{M} (A_{i,i-1} a_i^\dagger a_{i-1} + 1/2 B_i a_i^\dagger a_i) + q A_{1M} a_1^\dagger a_M + 1/2 B_1 a_1^\dagger a_1 + \text{H.c.} \tag{3}$$

It turns out that the partition function and correlators for the model can be calculated exactly, which should shed light on the whole problem.

First we describe and discuss our main results for the thermodynamical quantities associated with the Hamiltonian (3). We will outline the calculations at the end of the paper. The first result is the exact expression for the partition function of the system, $Z = \text{Tr}\exp[-\beta(H-\mu\hat{N})]$, at temperature $1/\beta$ and chemical potential μ, where $\hat{N} = \Sigma_{i=1}^{M} a_i^\dagger a_i$ is the number operator for q particles:

$$Z = \frac{1}{n}\sum_{l=0}^{n-1}\sum_{p=0}^{n-1} q^{-pl} Z_{p,l}, \quad Z_{p,l} = \prod_{k_l^m} (1 + q^p e^{\beta(\mu - \epsilon(k_l^m))}). \tag{4}$$

Here the notation $\epsilon(k_l^m)$ was introduced for the k_l^mth eigenvalue of the hopping matrix $||A_{ij}||$ on the circle with q^l periodic boundary conditions (which corresponds to the substitution of $q^l A_{1M}$ instead of A_{1M} in the hopping matrix). For the homogeneous chain ($A_{i,i-1} = \mathscr{A}$) these eigenvalues have the form

$$\epsilon(k_l^m) = B + 2A\cos(k_l^m), \quad k_l^m = \frac{2\pi}{M}(m - lr/n), \tag{5}$$

with $m = 0, \ldots, M-1$. Using expression (4) we immediately obtain the representation for the distribution function $n(\beta,\mu)$ of the q particles in terms of transmuted Fermi-Dirac (or Bose-Einstein) functions $f_q(x) = 1/[1+q^{-1}\exp(x)]$:

$$n(\beta,\mu) = \sum_{l=0}^{n-1}\sum_{p=0}^{n-1} q^{-pl} \sum_{k_l^m} f_{q^p}(\beta(\epsilon^l(k_l^m) - \mu)) Z_{p,l}/nMZ. \tag{6}$$

So we see that in Eq. (6) q-deformed Fermi-Dirac functions, with all allowed powers of the deformation parameter q, make contributions. Such functions naturally interpolate between the fermionic distribution function ($q=1$) and bosonic distribution function ($q=-1$). Moreover they pick up all q-periodic boundary conditions which also reflects the q exchange factor gained due to the permutation of particles via the loop.

In the same way simple exact results for correlation functions can be obtained. For example,

$$\langle a_1(\tau)a^{\dagger}_{L+1}(0)\rangle = \frac{e^{-\tau M(B-\mu)}}{nZ}\sum_{l=0}^{n-1}\sum_{p=0}^{n-1} q^{-lp}\mathrm{Det}C^l_p(\tau)(C^l_p(\tau))^{-1}_{1,L+1}, \quad (7)$$

where L is a relative coordinate and the matrix C is defined by the relation

$$C^l_p(\tau)_{m',m''} = \frac{1}{M}\sum_{k^m_{l+1}} e^{\tau(\epsilon(k^m_{l+1})-\mu)+ik^m_{l+1}(m'-m'')} + \frac{q^p}{M}\sum_{k^m_l} e^{(\tau-\beta)(\epsilon(k^m_l)-\mu)+ik^m_l(m'-m'')} \times[1+(q^{-1}-1)\theta(L-m')] \quad (8)$$

(here we used the lattice θ symbol which is continuous from the right). We checked our formulas for the cases of small M by straightforward calculations.

The note about picking up all q-periodic boundary conditions allows us to look at the problem from a different position. Indeed, from the original form of the Hamiltonian (3), which is quadratic in the creation (annihilation) operators, it is not difficult to see that, using the appropriate diagrammatic technique (for example in the q-field technique [4]), all contributions to the thermodynamical quantities will be given by vacuum diagrams with some exchange factors. And this does not depend on the space dimension. Let us now stress again one of our main results concerning the qXX model: the partition functions and correlation functions for a system with such the exchange statistics can be written as a double sum of terms indexed by all possible deformations of exchange factor and all permutation loops in the systems. This suggests that the theory may be reformulated as a theory of loops with weights defined by the deformed exchange factors. This may prompt an ansatz for the partition function in nD after the summation of contributions for different loops: sums over all loops in the configuration space, with all allowed q-periodic boundary conditions for them and all possible q deformations of Fermi-Dirac constructions.

In the particular case $q=-1$ the Hamiltonian (3) can be realized as a Hamiltonian of the spin-1/2 compact XX-chain in a magnetic field B (for the sake of simplicity we deal with the homogeneous case):

$$H=\sum_{i=2}^{M}(A_x s^x_i s^x_{i-1}+A_y s^y_i s^y_{i-1}-Bs^z_i)-B_1 s^z_1 + A_x s^x_1 s^x_M + A_y s^y_1 s^y_M + MB/2, \quad (9)$$

if we identify $A_x=A_y$ and the creation (annihilation) operators with spin upper (lower) operators as usual:

$$a_i=s^+_i=s^x_i-is^y_i, \quad a^{\dagger}_i=s^-_i=s^x_i+is^y_i. \quad (10)$$

After the introduction of anisotropy $A_{x(y)}=2(A\pm\gamma)$ the Hamiltonian (9) becomes the Hamiltonian of a spin-1/2 compact XY chain in the magnetic field B. In contrast to previous work, where quantities were calculated in thermodynamical limit [5–9], we obtain exact formulas for the partition function and correlators for the Hamiltonian of the XY model in compact lattice topology. In the thermodynamical limit statistical effects, which are proportional to the inverse size of the system, $1/M$, are negligible and the formulas of the paper are transformed into the known results. However, there is a field where boundary conditions *are relevant*. Recently a lot of attention was attracted by the theory of the so-called J aggregates, i.e., molecular aggregates with an unusually sharp absorption band ([10], [11] and references therein). The main advances were related with the use of the exact results for 1D chains. Frenkel excitons in such long aggregates obey the Paulionic commutation relations [12], or, in a more general case (if we take into account retardation effects [13]), q particle commutation relations. In the theory of the optical response and spectroscopy of long cyclic molecules the thermodynamical limit is not appropriate. On the other hand, the XY model recently arose in models of adsorption processes with diffusional relaxation [14]. Here the compact case is also interesting. The same can be said about the application of results to the theory of defectons where the statistics of defectons is exactly Paulionic statistics [15]. Let us again list the main results.

The partition function of the model $Z(\beta,B)$ contains four terms, two of which have a fermionic nature and the others have a bosonic ones:

$$Z=\tfrac{1}{2}(Z^+_f+Z^-_f+1/Z^+_b-1/Z^-_b). \quad (11)$$

Here $Z^{\pm}_f$ ($Z^{\pm}_b$) are fermionic (bosonic) partition functions,

$$Z^{\pm}_f=e^{-\beta BM/2}\prod_{k_\pm} e^{\beta E(k_\pm)/2}(1+e^{-\beta E(k_\pm)})$$

$$Z^{\pm}_b=e^{\beta BM/2}\prod_{k_\pm} e^{-\beta E(k_\pm)/2}/(1-e^{-\beta E(k_\pm)}),$$

for systems with the energy spectra,

$$E(k_\pm)=[B+2A\cos(k_\pm)]\sqrt{1+\frac{[2\gamma\sin(k_\pm)]^2}{[B+2A\cos(k_\pm)]^2}}$$

and antiperiodic (periodic) boundary conditions,

$$k_+=\frac{2\pi}{M}(m+1/2), \quad k_-=\frac{2\pi}{M}m, \ \ m=0,\dots,M-1.$$

We have also calculated correlation functions for various spin components. One of involved correlation functions is presented here. Using the mutipliers $g^{\pm}_k(\beta)=\mathrm{ch}\beta E_k\pm\cos\theta_k\mathrm{sh}\beta E_k$, $\theta_k=\arcsin(-2\gamma\sin k/E_k)$ and the matrix notations

$$D^{(1)}=\mathrm{diag}\left(\frac{1}{g_k^+(\beta-it)}\right),$$

$$B^{(1)}_{kk'}=-\delta_{k,-k'}\frac{\sin\theta_k\sinh(\beta-it)E_k}{2g_k^+(\beta-it)},$$

$$D^{(2)}=\mathrm{diag}\left(\frac{1}{g_k^-(it)}\right),\quad B^{(2)}_{kk'}=-\delta_{k,-k'}\frac{\sin\theta_k\sinh(itE_k)}{2g_k^-(it)},$$

$$(U_+)_{k_-k_+}=\frac{1}{M}\sum_{m=1}^{M}e^{im(k_+-k_-)},$$

$$(U_-)_{k_+k_-}=\frac{1}{M}\sum_{m=1}^{M}e^{im(k_--k_+)}$$

we have found $\langle a_1(t)a^\dagger_{L+1}(0)\rangle=(1/2Z)\{K_f^++K_b^++K_f^--K_b^-\}$, with

$$K^{\pm}_{f(b)}=(-1)^{\frac{M(M-1)}{2}}\mathcal{P}(G_\pm^{f(b)})e^{-\frac{\beta MB}{2}}\times\left(\prod_{k_\pm}g^+_{k_\pm}(\beta-it)\prod_{k_\mp}g^-_{k_\mp}(it)\right)^{1/2}\times\frac{1}{M}\sum_{k_\pm,k'_\pm}e^{ik'_\pm-ik_\pm(L+1)}\times(Q_\pm^{f(b)}+T_\pm^{f(b)}(Q_\pm^{f(b)})^{-tr}S_\pm)^{-1}_{k'_\pm k_\pm}. \tag{12}$$

Here $\mathcal{P}(G)$ is the Pfaffian of block matrix G,

$$G_\pm^{f(b)}=\begin{pmatrix}S_\pm & (Q_\pm^{f(b)})^{tr}\\ -Q_\pm^{f(b)} & T_\pm^{f(b)}\end{pmatrix}, \tag{13}$$

with blocks $Q_\pm^{f(b)}=W_\pm^{f(b)}D_\pm^{(1)}+U_\pm^+D_\mp^{(2)}U_\pm$, $T_\pm^{f(b)}=2\{W_\pm^{f(b)}B_\pm^{(1)}(W_\pm^{f(b)})^{tr}+U_\pm^+B_\mp^{(2)}U_\pm\}$, $S_\pm=-2\{B_\pm^{(1)}+U_\pm^{tr}B_\mp^{(2)}U_\pm\}$, and at the end

$$W^{f(b)}_{k,k'}=\pm\left(\delta_{k,k'}-2\frac{1}{M}\frac{\sin\frac{1}{2}(k'-k)L}{\sin\frac{1}{2}(k'-k)}e^{1/2\,i(k'-k)(L+1)}\right).$$

Indices "+" and "−" at matrices label the momentum space $\{2\pi(m+1/2)/M\}$ or $\{2\pi m/M\}$ in which these matrices are considered. For the case of $\gamma=0$ we return to Eq. (7) with $q=-1$ which was checked by computer symbolic calculations for small values of M. On the other hand, our numerics did not support the result of Ref. [10], where it was claimed that the formula for the correlator of the cyclic *XX* model was obtained. In the thermodynamical limit we produce results consistent with those of Ref. [8]

Now we outline the calculational procedure which leads to expressions (4) and (6) and then give the modification for the case of the *XY* model (9). To this end we apply to the creation (annihilation) operators $a_i^\dagger$ (a_i) the Jordan-Wigner transformation as in Ref. [5] for the case of the Paulion chain $(q=-1)$:

$$a_i=q^{\sum_{k=1}^{i}c_k^\dagger c_k}c_i,\quad a_i^\dagger=c_i^\dagger q^{-\sum_{k=1}^{i}c_k^\dagger c_k}. \tag{14}$$

Here $c_i^\dagger,(c_i)$ are the creation (annihilation) operators of spinless fermions at the ith site. The operator (3) is cast in the form

$$H=\sum_{i=2}^{M}(A_{i,i-1}c_i^\dagger c_{i-1}+1/2B_ic_i^\dagger c_i)+A_{1M}q^{\hat N}c_1^\dagger c_M+1/2B_1c_1^\dagger c_1+\text{H.c.}, \tag{15}$$

where $\hat N=\Sigma_{i=1}^{M}c_i^\dagger c_i$ is the number operator of the fermions. To proceed we introduce the set of operators $\{P_l\}_{l=0}^{n-1}$ which are projection operators on the subspaces of $l(\mathrm{mod}n)$ particles:

$$P_l=\frac{1}{n}\sum_{p=0}^{n-1}q^{-lp}q^{\hat Np}. \tag{16}$$

Making use of these projection operators with the obvious property $\Sigma_{l=0}^{n-1}P_l=I$ we then obtain the following representation for the partition function $Z=\mathrm{Tr}\exp[-\beta(H-\mu\hat N)]$:

$$Z=\sum_{l=0}^{n-1}\mathrm{Tr}\exp[-\beta(H-\mu\hat N)]P_l, \tag{17}$$

which allows us to replace in each term of the sum (17) the multiplier q^N in the Hamiltonian (15) by the numerical constant q^l. Moreover, since H and $\hat N$ commute, each pth term of the expression (16) for the projection operators can be taken into account by a shift of the chemical potential μ to the value $\mu^{(p)}=\mu+2\pi ipr/n\beta$. This leads to the representation for the partition function,

$$Z=\frac{1}{n}\sum_{l=0}^{n-1}\sum_{p=0}^{n-1}q^{-lp}\mathrm{Tr}\exp[-\beta(H^{(l)}-\mu^{(p)}\hat N)], \tag{18}$$

where $H^{(l)}$ are q^l-periodical square fermionic Hamiltonians. After making use of the standard results for the partition function of a free fermion system we regain Eq. (4). The calculation of the correlation function is more cumbersome but straightforward as well.

Up to this point we did not use the functional integral approach. However, it allows us to look at the problem from another viewpoint and, furthermore, it is closely connected with the modification of the calculations for the case of the *XY* chain. Indeed, each term of the sum (18) can be represented in the form of a functional integral,

$$\mathrm{Tr}\exp[-\beta(H^{(l)}-\mu^{(p)}N)]=\int D\overline{\xi(\tau)}D\xi(\tau)e^{S_{lp}}$$

over the Grassmann fields $\overline{\xi(\tau)},\xi(\tau)$ with antiperiodic boundary conditions $\bar\xi(\beta)=-\bar\xi(0)$, $\xi(\beta)=-\xi(0)$ and the action

$$S_{lp}=\int_0^\beta d\tau\left\{\bar\xi\frac{\partial\xi}{\partial\tau}-H^{(l)}(\bar\xi,\xi)+\mu\bar\xi\xi\right\}+\int_0^\beta d\tau\frac{2\pi ipr}{n\beta}\bar\xi\xi\equiv S_l+\delta S_p. \tag{19}$$

Under the change of variables $\overline{\xi(\tau)} \to \overline{\xi(\tau)} e^{-i(2\pi pr/n\beta)\tau}$, $\xi(\tau) \to \xi(\tau) e^{i(2\pi pr/n\beta)\tau}$, the last term of the previous expression, δS_p, disappears, which, however, is compensated by changing the boundary conditions for the fields of integration,

$$\overline{\xi(\beta)} = -q^{-p}\overline{\xi(0)}, \quad \xi(\beta) = -q^{p}\xi(0) \tag{20}$$

(a procedure of this type was used in Ref. [16] to construct the Feynman diagram technique for spin systems). As a result we reach the following functional integral representation of the partition function:

$$Z = \sum_{p=0}^{n-1}\sum_{l=0}^{n-1} q^{-lp}\int D\overline{\xi(\tau)} D\xi(\tau) e^{S_l}/n, \tag{21}$$

provided with the q^p-periodic boundary conditions (20). In this form the equation turns out to be valid for the case of the *XY* model for spin-1/2, although the justification needs to attract other ideas.

Let us clarify the problem arising in the case of the *XY* model. Indeed, after the Jordan-Wigner transformation (14) the Hamiltonian (9) becomes the operator,

$$H = \sum_{i=2}^{M} (A c_i^\dagger c_{i-1} + \tfrac{1}{2} B_i c_i^\dagger c_i + \gamma c_i^\dagger c_{i-1}^\dagger) + \tfrac{1}{2} B_1 c_1^\dagger c_1 - A(-1)^{\hat{N}} c_1^\dagger c_M - \gamma(-1)^{\hat{N}} c_1^\dagger c_M^\dagger + \text{H.c.}, \tag{22}$$

which differs from the Hamiltonian (15) by additional terms with the anisotropy parameter γ. They cause the Hamiltonian to no longer commute with the number operator for particles $\hat{N}$, which does not allow us to use the device of shifting the chemical potential. However the Hamiltonian still commutes with the operator $\tau = (-1)^{\hat{N}}$. This leads to the formula, which is analogous to Eq. (18),

$$Z = \tfrac{1}{2}(\text{Tr}e^{-\beta H^{(+)}} + \text{Tr}e^{-\beta H^{(-)}} + \text{Tr}\tau e^{-\beta H^{(+)}} - \text{Tr}\tau e^{-\beta H^{(-)}}), \tag{23}$$

where $H^{(\pm)}$ coincide with the original Hamiltonian after the substitution $\tau = (-1)^{\hat{N}} \to \pm 1$. Although the last two terms cannot be calculated by changing the chemical potential, taking into account τ in them is also achieved by changing boundary conditions (20). This was demonstrated in Ref. [17] in the framework of supersymmetric quantum mechanics, where the operators τ and $\text{Tr}\tau e^{-\beta H}$ play the role of supersymmetric involution and supersymmetric Witten index of the Hamiltonian H. That is why we term this the *supersymmetric trick*.

All of this returns us to Eq. (21) with $q = -1$, which after the use of the Bogoliubov transformation for the variables of integration leads to formula (11). We should mention that the same trick can be used to calculate correlation functions.

In conclusion, we calculated exactly the partition functions and correlators for systems of free particles with q-deformed exchange statistics and the spin-1/2 *XY* model on a compact chain with periodic boundary conditions. We demonstrated that the deformation of the statistics can be taken into account by changing the boundary conditions for the fields of integration in the functional integral framework that leads to the transmutation of distribution functions. In such a way deformed Fermi-Dirac functions appeared. We also stated a conjecture about the form of thermodynamical quantities in higher dimensions.

We wish to thank V. M. Agranovich, J. M. F. Gunn, and A. S. Stepanenko for useful discussions. This work was supported by the Russian Fund of Fundamental Investigations, Grant No. 95-01-00548 and partially (K.I.) by the U.K. EPSRC under Grant No. GR/J35221, Euler stipend of German Mathematical Society and Grant No. INTAS-939.

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