A Generalization of Quantum Statistics

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Abstract

We propose a new fractional statistics for arbitrary dimensions, based on an extension of Pauli's exclusion principle, to allow for finite multi-occupancies of a single quantum state. By explicitly constructing the many-body Hilbert space, we obtain a new algebra of operators and a new thermodynamics. The new statistics is different from fractional exclusion statistics; and in a certain limit, it reduces to the case of parafermi statistics.

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The thermodynamics of a macroscopic system is determined microscopically by the statistics of its constituent particles and elementary excitations. Herein lies a fundamental significance of statistics. Ever since Heisenberg's second paper on matrix mechanics, it has been known that a many-body wavefunction is symmetric under permutations of identical bosons, but it is antisymmetric for identical fermions. The corresponding commutation and anticommutation relations bilinear in field operators result in bose and fermi statistics respectively. Particles are accordingly classified into bosons and fermions. The overriding difference between the two groups is that bosons condense while fermions exclude. But it is natural to inquire whether there are any meaningful generalizations of statistics intermediate between these two.

Attempts to generalize statistics dates back at least to Green's work in 1953 [1][2]. Green found that the principles of quantum mechanics also allow two kinds of statistics called parabose statistics and parafermi statistics of positive integral order M (the M=1 cases reduce to the familiar Bose-Einstein statistics and Fermi-Dirac statistics respectively). They are described by trilinear commutation relations among the creation and annihilation operators. Subsequently, the case of non-integral M was investigated for possible deviations from Bose and Fermi statistics, and in particular, for possible violations of Pauli's exclusion principle [3][4]. This saga culminated with a recent study of infinite statistics [5] in which all representations of the symmetric group can occur; this case is realized by the q-mutator algebras.

Another type of interpolating statistics, spearheaded by Wilczek, is provided by the concept of anyons [6]. Anyons are particles whose wavefunctions acquire an arbitrary phase when two of them are braided; they obey fractional statistics. More recently, Haldane introduced another definition of statistics based on a generalization of the Pauli principle [7][8]. Unlike the anyon fractional exchange statistics which is meaningful only in two spatial dimensions, Haldane's fractional exclusion statistics is formulated in arbitrary dimensions. The thermodynamics based on exclusion statistics is studied in Ref.[8]. The issue whether anyons obey fractional exclusion statistics

in the framework of quantum field theory is addressed in Ref.[9]. In this Letter we introduce another type of statistics which is based on a (different) logical extension of the Pauli principle. In the new statistics, we allow for multi-occupancy of a single quantum state by up to a maximum number M of identical particles. The M = 1 case yields the conventional Fermi statistics while the M $\to \infty$ case corresponds to the conventional Bose statistics. The new statistics bears some resemblance to fractional exclusion statistics but is distinct from it.

In the literature a frequently used approach to study the quantum features of (especially fermi and fermi-like) many-body systems is to start with assumptions of commutation relations among certain operators. In this letter, we would like to start with the construction of Hilbert space of quantum states and then "derive" some relations of the operators. Consider the Hilbert space spanned by the eigenstates of the particle number operator $\hat{N}$, $\{|j>, \ j = 0, 1, 2, \cdots\}$. The j-particle state $|j>$ satisfies

$$\hat{N}|j>= j|j> , \qquad <j|k>= \delta_{jk} . \tag{1}$$

Obviously, the ground state is the zero-particle state $|0>$. We define the one-particle state as a superposition of M single states $|e_i>$:

$$|1>= c_1 c_2 \cdots c_{M-1}|e_1> +s_1 c_2 \cdots c_{M-1}|e_2> + \cdots +s_{M-1}|e_M> , \tag{2}$$

where $c_i = \cos\theta_i$, $s_i = \sin\theta_i$, $\theta_i \neq 0$, or multiples of $\pi/2$. The use of the angles is just a matter of convenience. In this case, the one-particle state can be thought of as a unit vector on a (M$-$1)-sphere. The M single states $|e_i>$, $i = 1, 2, \cdots$ M, satisfy

$$< e_i|e_j >= \delta_{ij} , \quad \text{and} \ \ (|e_i>)^2 = 0 . \tag{3}$$

The latter condition can be understood as a reflection of the Pauli exclusion principle, namely, a two-$|e_i>$ state is forbidden.

The two-particle state is defined as a superposition of the tensor products

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$$|e_i > |e_j >$$

$$|2 >= \sum_{i<j}^{\mathrm{M}} c_{ij}|e_i > |e_j > . \qquad (4)$$

Similarly, three and more particle states can be defined as a superposition of tensor products $|e_i > |e_j > |e_k >$ with c-number coefficients c_{ijk} and so on. How to determine c_{ij}, c_{ijk} and so on, in term of the angles θ_i, will be discussed later. We should emphasize that in a tensor product of single states, we adopt the rule that the order of single states does not make a difference, $i.e.$ $|e_i > |e_j >= |e_j > |e_i >$. Due to the second condition in Eq.(3), the M-particle state

$$|\mathrm{M} >= \prod_{i=1}^{\mathrm{M}} |e_i > , \qquad (5)$$

is the maximal-particle state, the state with the maximum number of M particles. There are no states beyond it, $i.e.$ states $|j >$ for $j > \mathrm{M}$ do not exist.

Now, we introduce the annihilation and creation operators, a and $a^\dagger$,

$$a|j >= f_j|j - 1 > , \quad a^\dagger|j >= f_{j+1}^*|j + 1 > . \qquad (6)$$

In particular, $a|0 >= 0$ and $a^\dagger|0 >= |1 >$. Hereafter we choose f_1 and all f_j to be real for convenience (this does not affect the physics we will discuss in the single particle species case). One can readily check the following commutation relation of $\hat{N}$ with a and $a^\dagger$

$$\hat{N}a - a\hat{N} = -a , \quad \text{and} \quad \hat{N}a^\dagger - a^\dagger\hat{N} = a^\dagger . \qquad (7)$$

Starting from the one-particle state Eq.(2), using the relation

$$(a^\dagger)^j|0 >= (|1 >)^j \sim |j > , \quad \text{or} \quad a^j|j >\sim |0 > , \qquad (8)$$

the normalization condition in Eq.(1), and $f_0 = 0$ and $f_1 = 1$, one can systematically determine the amplitude f_2 and the coefficients c_{ij}, f_3 and c_{ijk}, and so on, set by set. To be concrete, let us take M = 2 and 3 as examples. For M = 2, the one-particle state is $|1 >= c|e_1 > +s|e_2 >$. Acting the creation operator $a^\dagger$ on $|1 >$, one has

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$a^\dagger|1>=(|1>)^2=2cs|e_1>|e_2>=f_2|2>$. Therefore $f_2=2\cos\theta\sin\theta$. Obviously $|2>$ is the maximal-particle state since $|3>=0$. This is tantamount to $f_j=0$ for $j>2$, or equivalently $(a^\dagger)^3=a^3=0$.

For M $=3$, the one-particle state is $|1>=c_1c_2|e_1>+s_1c_2|e_2>+s_2|e_3>$. From $a^\dagger|1>=(|1>)^2=f_2|2>$, we obtain $f_2=2s_1c_1c_2^2\sqrt{1+t_2^2/s_1^2c_1^2}$ with $t_2=\tan\theta_2$ and $|2>=1/\sqrt{1+t_2^2/s_1^2c_1^2}(|e_1>|e_2>+t_2/s_1|e_1>|e_3>+t_2/c_1|e_2>|e_3>)$. Using $a^\dagger|2>=f_3|3>$ with $|3>=|e_1>|e_2>|e_3>$, we readily obtain $f_3=3s_2/\sqrt{1+t_2^2/s_1^2c_1^2}$. The amplitudes $f_j=0$ for $j>3$, equivalently $(a^\dagger)^4=a^4=0$.

Let us consider the operator algebra of a and $a^\dagger$. First, for a general M, there are no simple bi-linear operator relations like $[a,a^\dagger]_\pm=1$ that the conventional boson and fermion operators satisfy. Instead, here we have

$$(aa^\dagger+a^\dagger a)|j>=(f_j^2+f_{j+1}^2)|j> . \qquad (9)$$

For M $=1$, we recover the anti-commutation relation for fermions.

For any given M, $a^j=(a^\dagger)^j=0$ only if $j>$ M. Therefore, there exist (M+1)-linear relations between a and $a^\dagger$. For example, for M $=2$, one has the cubic relations

$$a^2a^\dagger+f_2^2a^\dagger a^2 = f_2^2a , \qquad (10)$$
$$a^2a^\dagger+a^\dagger a^2+aa^\dagger a = \text{Tr}(aa^\dagger)a , \qquad (11)$$

where $\text{Tr}(aa^\dagger)=\sum_{j=1}^M f_j^2$, plus the hermitian conjugate relations.

For M $=3$, there are the quartic relations like

$$a^3a^\dagger+f_3^2a^\dagger a^3 = f_3^2a^2 , \qquad (12)$$
$$a^3a^\dagger+a^\dagger a^3+a^2a^\dagger a+aa^\dagger a^2 = \text{Tr}(aa^\dagger)a^2 , \qquad (13)$$

plus the hermitian conjugate relations. We speculate that the multi-linear relations among a and $a^\dagger$ in the limit M $\to\infty$ (and with a suitable choice of the theta angles) actually reduce to the bilinear commutation relation for Bose statistics.

Next we consider the particle number operator $\hat{N}$ in terms of the creation and annihilation operators $a^\dagger$ and a. One way to do this is to ssume, for a given M,

$$\hat{N} = C_1 a^\dagger a + C_2 (a^\dagger)^2 a^2 + \cdots + C_M (a^\dagger)^M a^M . \tag{14}$$

Then the M coefficients C_j, $j = 1, 2, \cdots, M$, can be determined by using the M independent equations $\hat{N}|k> = k|k>$, $k = 1, 2, \cdots, M$. For example, for M = 2: $C_1 = 1$ and $C_2 = (2 - f_2^2)/f_2^2$. For M = 3: $C_1 = 1$, $C_2 = (2 - f_2^2)/f_2^2$, and $C_3 = (3/f_3^2 - 3 + f_2^2)/f_2^2$.

The particle number operator $\hat{N}$ can be expressed in other forms for certain values of the theta angles. For example, if the θ_i's in Eq.(2) are chosen so that the one particle state is $|1> = 1/\sqrt{M} (|e_1> + |e_2> + \cdots |e_M>)$ and if the operators a and $a^\dagger$ are replaced by operators $b/\sqrt{M}$ and $b^\dagger/\sqrt{M}$, the particle number operator takes the form $\hat{N} = \frac{1}{2}(b^\dagger b - bb^\dagger) + \frac{M}{2}\mathbf{1}$. This latter form was used in the study of parafermi statistics [1][2].

With the Hilbert space of quantum states for the new statistics and the diagonal particle number operator now available, it is natural and straightforward to consider the quantum statistical mechanics of a system that is compatible with such a construction (note that systems of this kind are not necessarily described by a free theory).

Let us assume a single particle to have energy $\epsilon = \epsilon(\mathbf{p})$, then the Hamiltonian operator takes the form

$$\hat{H} = \epsilon \hat{N} . \tag{15}$$

The energy spectrum of the system for a given M is given by $\{\epsilon,\ 2\epsilon,\ \cdots,\ M\epsilon\}$, similar to that for a spin system in a magnetic field.

The grand partition function is

$$Z = \mathrm{Tr} e^{-\beta(\hat{H} - \mu\hat{N})} = \sum_{j=0}^{M} <j|e^{-\beta(\hat{H} - \mu\hat{N})}|j> = \prod_{\mathbf{p}} \sum_{j=0}^{M} (z e^{-\beta\epsilon})^j , \tag{16}$$

where β is the reciprocal of temperature T, μ is the chemical potential, the fugacity is $z = e^{\beta\mu}$, and the Boltzmann constant is $k_B = 1$. For M = 1, $Z = \prod_{\mathbf{p}}(1 + z e^{-\beta\epsilon})$

is the partition function for free fermions; while for M $= \infty$, $Z = \prod_{\mathbf{p}} 1/(1 - ze^{-\beta\epsilon})$ recovers the partition function of free bosons [10]. For M $\neq 1$ and ∞, Z describes a system interpolating between free fermions and free bosons. Note that the resulting thermodynamics is insensitive to the particular values of the set of amplitudes f_j. In particular, for the M $= 2$ case, even when the one-particle state $|1>$ is predominantly $|e_1>$ or $|e_2>$, the statistics is very different from Fermi statistics, suggesting that the models discussed in Ref.[3] do not yield weak violations of the Pauli principle as correctly pointed out in Ref.[4].

With the grand partition function Z, one can calculate various thermodynamical quantities. The particle number

$$N = z\frac{\partial}{\partial z}\ln Z = \sum_{\mathbf{p}} \frac{\sum_{j=1}^{M} j(ze^{-\beta\epsilon})^j}{\sum_{j=0}^{M}(ze^{-\beta\epsilon})^j} \ . \tag{17}$$

Accordingly, the average occupation numbers are

$$n(\epsilon) = \frac{\sum_{j=1}^{M} j(ze^{-\beta\epsilon})^j}{\sum_{j=0}^{M}(ze^{-\beta\epsilon})^j} \ . \tag{18}$$

At $T = 0$, $n(\epsilon) = 0$ for $\epsilon > \mu$; while $n(\epsilon) = $ M for $\epsilon < \mu$. The fermi energy ϵ_F is defined by the particle density $n = N/V = (1/V)\sum_{\mathbf{p}<\mathbf{p}_F} n(\epsilon)$ at absolute zero. As $T \to \infty$, $n(\epsilon) = $ M$/2$.

One can also calculate the entropy S by applying $S = -\partial F/\partial T$, where $F = -T\ln Z$ is the grand potential. Using Eq.(18) to invert $ze^{-\beta\epsilon}$ in term of the average occupation number $n(\epsilon)$ one can then express S in term of $n(\epsilon)$. For example, for M $= 2$, we find

$$S = \sum_{\mathbf{p}} \left(-\ln n(\epsilon) + (1 - n(\epsilon))\ln x + \ln(1 + 2x)\right) \ , \tag{19}$$

where $x = (\sqrt{1 + 6n(\epsilon) - 3n^2(\epsilon)} - 1 + n(\epsilon))/2(2 - n(\epsilon))$.

The equation of state is given by

$$\beta PV = \ln Z = \sum_{\mathbf{p}} \ln \sum_{j=0}^{M}(ze^{-\beta\epsilon})^j \ , \tag{20}$$

where P denotes the pressure and V the volume. In the large volume ($V \to \infty$) limit, we replace the sum over momentum $\mathbf{p}$ by the integral over $\mathbf{p}$: $\sum_{\mathbf{p}} \to V \int d^D\mathbf{p}/(2\pi)^D$.

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Such a replacement is clearly valid only if the summand is finite for all $\mathbf{p}$. For the bose gas (the limit of $M \to \infty$), the summand $-\ln(1 - ze^{-\beta\epsilon})$ in Eq.(20) diverges as the fugacity $z \to 1$, because the single term corresponding to $\mathbf{p} = 0$ diverges. This is of course related to the Bose-Einstein condensation. On the other hand, for any finite M, the summand in Eq.(20) is finite for any value of $\epsilon(\mathbf{p})$.

In all our discussions so far we have made no reference to any specific spatial dimensions. We now consider a planar system. Furthermore, we assume the single particle energy ϵ take the form $\epsilon(\mathbf{p}) = \mathbf{p}^2/(2m)$, with m being the (effective) mass of the particles or excitations so that the system is an ideal gas. Using Eq.(20) and Eq.(17), and performing the integrations over $\mathbf{p}$, we readily obtain

$$\beta P = \frac{1}{\lambda^2} \sum_{k=1}^{\infty} \frac{z^k}{k^2} \left(1 - \frac{z^{Mk}}{M+1} \right) \qquad (z \leq 1), \quad (21)$$

$$= \frac{1}{\lambda^2} \left[\frac{\pi^2}{3} \frac{M}{M+1} + \frac{M}{2} (\ln z)^2 - \sum_{k=1}^{\infty} \frac{z^{-k}}{k^2} \left(1 - \frac{z^{-Mk}}{M+1} \right) \right] \qquad (z \geq 1), \quad (22)$$

$$n = \frac{N}{V} = \frac{1}{\lambda^2} \ln \frac{1 - z^{(M+1)}}{1 - z} , \qquad (23)$$

where $\lambda = \sqrt{2\pi\beta/m}$ is the thermal wavelength. Solving for z in Eq.(23) and substituting it into Eq.(21), in the high temperature and low density limit, i.e. $\lambda^2 n \ll 1$, we can conduct a virial expansion in the form $\beta P = n \left(1 + B_2 \lambda^2 n + B_3 (\lambda^2 n)^2 + \cdots \right)$. For M = 2, we find $B_2 = -1/4$, $B_3 = 25/36$, $\cdots$; and for M = 3, $B_2 = -1/4$, $B_3 = 1/36$, $\cdots$. Actually from Eq.(21) and Eq.(23), it is not difficult to check that for any M > 1, the second virial coefficient is $-1/4$, the same as for the ideal bose gas (M = ∞). It implies that (for sufficiently small $\lambda^2 n$) the quantum effect on the ideal gas, for all M except M = 1, is equivalent to an attractive "interaction" among excitations. For ideal fermi gas (M = 1) this effect is a repulsive one as $B_2 = +1/4$.

In the low temperature and high density limit, i.e. $\lambda^2 n \gg 1$, most particles are in the states with energy $\epsilon < \epsilon_F = 2\pi n/Mm$. Using $U = F + TS + \mu N$, we obtain the internal energy

$$U = \frac{1}{2} N\epsilon_F \left(1 + \frac{2\pi^2}{3(M+1)} (\frac{T}{\epsilon_F})^2 + \cdots \right) . \qquad (24)$$

The first term is the ground state energy, a result that can be verified by using $\sum_{\mathbf{p}<\mathbf{p}_F} M p^2/(2m) = N\epsilon_F/2$. From the above equation the specific heat at constant volume can be readily found: $C_V/N \simeq \frac{2\pi^2}{3(M+1)}\frac{T}{\epsilon_F}$. These suggest that in the low temperature and high density limit, a system in which each quantum state has a maximum multi-occupancy of $M < \infty$ is like the fermion system ($M = 1$).

A comparison of the quantum statistical mechanics obtained here with that for exclusion statistics can now be made. Both fractional statistics, based on general-izations of Pauli's exclusion principle, are well defined in arbitrary dimensions. At zero temperature, the $n(\epsilon)$ distributions in the two thermodynamics are the same if the statistical parameter g in exclusion statistics is identified with $1/M$ in the new statistics. But there are profound differences between the two statistics. The second virial coefficient for a free planar exclusion statistical system, such as the free anyon system, is given by $B_2 = 1/4 - g/2$ (where $g = 0, 1$ for fermion and boson statistics respectively) [8][9]. Accordingly the statistical interaction is attractive, neutral, or repulsive, depending on the value of g. In particular, for semions with $g = 1/2$, it is neutral (to this order); and for others with fractional $g = 1/M$ ($M > 2$), it is repulsive. In contrast, we find an attractive interaction for all $M > 1$ in the new statistics discussed above. Moreover, the particle distribution $n(\epsilon)$ are in general very different in the two statistics. For example, the distribution of semions from the exclusion statistical derivation takes the form [8]: $n(\epsilon) = 1/\sqrt{1/4 + e^{2\beta\epsilon}/z^2}$. This is different (except at zero temperature) from the one given by Eq.(18) for $M = 2$, $n(\epsilon) = (2 + e^{\beta\epsilon}/z)/(1 + e^{\beta\epsilon}/z + e^{2\beta\epsilon}/z^2)$. Integrating out the distributions over ϵ, we find the resulting densities are different too. The statistical weights W for fractional exclusion statistics are also quite different from those for the new statistics. For instance, for N identical semions occupying G states, it reads $W = \begin{pmatrix} G + \frac{1}{2}(N-1) \\ N \end{pmatrix}$ in exclusion statistics [7][8], whereas for $M = 2$ in the new statistics we obtain

$$W = \sum_0^{[\frac{N}{2}]} \begin{pmatrix} N-k \\ k \end{pmatrix} \begin{pmatrix} G \\ N-k \end{pmatrix}, \tag{25}$$

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where $[\frac{N}{2}]$ denotes $N/2$ and $(N-1)/2$ for $N=$ even and odd, respectively. We conclude that the statistics associated with multi-occupancy of a single quantum state and the resulting operator algebra are different from the exclusion statistics defined in Ref.[7] (in contrast to a recent proposal [11], in which the exclusion statistical parameter g is assumed to be connected to the maximum occupancy number M by $g=1/M$ and the statistical distributions in exclusion statistics are connected to the amplitudes f_j).

Note added: After this paper was completed, we noticed a recent interesting work [12], in which an issue relevant to this paper was also addressed.

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