Fractional Exclusion Statistics and Two Dimensional Electron Systems

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Using the Thomas-Fermi approximation, we show that an interacting two dimensional electron gas may be described in terms of fractional exclusion statistics at zero and finite temperatures when the interaction has a short-range component. We argue that a likely physical situation for this phenomenon to occur may exist in two dimensional quantum dots.

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Fractional exclusion statistics or the generalized exclusion principle was first proposed by Haldane [1,2] in the context of excitations in spin chains. Experimentally, the best evidence comes from recent neutron inelastic scattering experiment [3] on the compound $KCuF_3$, which is a one dimensional Heisenberg antiferromagnet above 40 K. The observed inelastic scattering is best fitted by spinon excitations in a spin chain whose pairwise interaction falls off as the inverse square of the lattice distance [4]. The dynamic correlation function for such a system has been calculated by Haldane and Zirnbauer [5]. The concept of fractional exclusion statistics has been generalized to the case of a gas of particles [6] defined by a distribution function [7,8] that allows for partial or multiple occupancy of a single-particle state. In principle, the statistics is applicable to particles in any spatial dimension, but most known examples are mathematical models in one dimension [9-11] with a pairwise inverse-square interaction. The first calculation for a two dimensional realistic system in this context was done by Johnson and Canright [12], who demonstrated, by exact diagonalization of a small number of interacting electrons, that the bulk excitations in fractional quantum Hall effect (FOHE) liquids exhibit Haldane statistics. In this paper, we show that under certain conditions a two dimensional interacting electron gas in its ground state may exhibit these statistics. The conditions are shown to be favorable for electrons in a quantum dot. In this case, it is shown that the dominant effect of the interaction may be incorporated in the fractional statistics of the gas. If the residual interactions are neglected, then the system also obeys Haldane statistics at finite temperature. This opens up the exciting possibility that the bulk properties of a mesoscopic two dimensional system may be understood by regarding it as an almost ideal fractional statistics gas confined in a potential well.

The claims made in this paper are based on the Thomas-Fermi (TF) method [13]. Being a mean-field method, it cannot reproduce two-body correlations, but is successful in giving a good estimate of bulk properties like the ground-state energy and the single-particle spatial density. It has previously been applied with success to atoms [14], nuclei [15], and metal clusters [16]. In two dimensions, TF yields an accurate approximation to the total energy of a many-anyon system [17]. For an ideal gas obeying the generalized exclusion statistics, TF calculation has been shown to yield the exact answer for the energy in the large-N limit [18]. It is therefore reasonable to expect that the method gives meaningful answers. We start by constructing the energy density functional for the groundstate energy of a system of interacting spin-half fermions. Consider the *N*-fermion Hamiltonian in two dimensions,

$$H = \frac{1}{2m^*} \sum_{i=1}^{N} p_i^2 + \sum_{i=1}^{N} V_1(r_i) + \sum_{j \le k} V_2(|\vec{r}_j - \vec{r}_k|),$$
(1)

where V_1 is a one-body confining potential whose specific form is not crucial at present and V_2 is the two-body potential that is repulsive. In a mean-field theory, the expression for the energy at zero temperature is given by

$$E = \int d^2r \left[\frac{\hbar^2}{2m^*} \tau(r) + V_1(r)\rho(r) + \frac{1}{2} \left\{ \rho(r) \int d^2r' \,\rho(r') V_2(|\vec{r} - \vec{r}'|) - C \int d^2r' \,|\rho(r,r')|^2 V_2(|\vec{r} - \vec{r}'|) \right\} \right],$$
(2)

where $\rho(r)$ is the spatial single-particle density, $\tau(r)$ is the kinetic energy density, and $\rho(r, r')$ is the density matrix. In the above we have taken into account the effect of both direct and exchange terms in the interaction energy. The factor 1/2 is the correction due to the overcounting of pairs. The constant *C* is determined by the spin polarization of the gas: for unpolarized electrons, it is 1/2, whereas for a fully polarized system, it is 1. For arbitrary polarization

 $P = (N_+ - N_-)/N$, where N_{\pm} is the number of up or down spins, the factor C = (1 + |P|)/2. The spatial density is normalized such that $N = \int d^2r \rho(r)$. In the Thomas-Fermi method, the kinetic energy density $\tau(r)$ is itself expressed in terms of the density $\rho(r)$ and its gradients. The energy and the density are determined selfconsistently by a variational principle. In two dimensions, the TF expression is $\tau(r) = \pi \rho^2(r)$, taking into account the spin-degeneracy factor of 2. In this case, there is no gradient correction in the bulk up to $O(\hbar^2)$. However, there are edge corrections when the sample is of finite size [19].

Next consider the energy due to the two-body interactions. The matrix element of the direct term is

$$\sum_{i,j} \langle ij | V_2 | ij \rangle = \int \rho(r_1) \rho(r_2) V(|\vec{r}_1 - \vec{r}_2|) d^2 r_1 d^2 r_2,$$
(3)

where the sum (here as well as in what follows) is over the *occupied single-particle states* only. The matrix element

of the exchange term is

$$\sum_{i,j} \langle ij | V_2 | ji \rangle = \int |\rho(r_1, r_2)|^2 V(|\vec{r}_1 - \vec{r}_2|) d^2 r_1 d^2 r_2,$$
(4)

where $\rho(r_1, r_2) = \sum_i \psi_i^*(r_1)\psi_i(r_2)$. At this stage, it is useful to perform the density-matrix expansion following Skyrme [20]. Defining $\vec{r} = \vec{r}_1 - \vec{r}_2$ and $\vec{R} = (\vec{r}_1 + \vec{r}_2)/2$ and expanding the density up to this order in \vec{r} , we obtain

$$\rho(\vec{r}_1) = \rho(\vec{R} + \vec{r}/2) = \rho(\vec{R}) + \frac{1}{2}(\vec{r} \cdot \nabla)\rho + \frac{1}{8}(\vec{r} \cdot \nabla)^2\rho + \cdots .$$
(5)

The direct matrix element may then be written as

$$\sum_{i,j} \langle ij | V_2 | ij \rangle = \int d^2 r \, V_2(r) \int d^2 R \, \rho^2(R) - \frac{1}{4} \int d^2 r \, r^2 V_2(r) \int d^2 R \, [\nabla \rho(R)]^2 + \cdots \,. \tag{6}$$

Similarly the density matrix $\rho(\vec{r}_1, \vec{r}_2)$ may be expanded up to second order in \vec{r} about \vec{R} , and on angle averaging

$$\rho(\vec{r}_1, \vec{r}_2) = \sum_i \psi_i^*(\vec{R} + \vec{r}/2)\psi_i(\vec{R} - \vec{r}/2) = \sum_i \left[\psi_i^*(\vec{R})\psi_i(\vec{R}) + \frac{1}{16}r^2(\psi_i^*\nabla^2\psi_i + (\nabla^2\psi_i^*)\psi_i - 2\nabla\psi_i^*\cdot\nabla\psi_i)\right], \quad (7)$$

and the exchange contribution to second order is given by

$$\sum_{i,j} \langle ij|V_2|ji\rangle = \int d^2r \, V_2(r) \int d^2R \, \rho^2(R) - \frac{1}{2} \int d^2r \, r^2 V_2(r) \int d^2R \, \tau(R)\rho(R) + \cdots \,. \tag{8}$$

Here the kinetic energy density is defined as

$$\tau = -\frac{1}{4} \sum_{i} [\psi_{i}^{*}(\nabla^{2}\psi_{i}) + (\nabla^{2}\psi_{i}^{*})\psi_{i}] + \frac{1}{2} \sum_{i} (\nabla\psi_{i}^{*}) \cdot (\nabla\psi_{i}).$$
(9)

Often the kinetic energy density is defined either by the first term or by the second term in the above equation without the overall 1/2. What we naturally get in the expansion is an average of both these commonly used forms. We have computed each one of these forms exactly using harmonic oscillator wave functions for a few particles. While the first and second terms show oscillations around the smooth TF density, the definition given above almost precisely coincides with the TF density even with as few as two particles.

We note that the leading terms in both direct and exchange terms are the same (proportional to ρ^2). For spin-half fermions the interaction energy is given by

$$\sum_{i,j} [\langle ij|V_2|ij\rangle - \delta_{m_i,m_j} \delta_{m_j,m_i} \langle ij|V_2|ji\rangle], \quad (10)$$

where m_i is the spin projection. Summing over all particle indices immediately gives a factor (1 + |P|)/2 for the exchange contribution, where *P* is the spin polarization of the system. Therefore, if there is no other degree of freedom, or if the spins are all polarized, the contribution from the leading terms to the interaction energy vanishes as it happens in FQHE systems. However, for the unpolarized 2D electron systems there is a factor of $\frac{1}{2}$ for exchange contribution. Here we concentrate on the unpolarized case. Combining all the contributions the total

energy of the system is given by

$$E = \int d^2r \left[\frac{\hbar^2}{2m^*} \pi \rho^2(r) + V_1(r)\rho(r) + \frac{1}{4} \rho^2(r)M_0 + \frac{1}{8} \{\pi \rho^3(r) - [\nabla \rho(r)]^2\}M_2 + \cdots \right],$$
(11)

where $M_n = \int d^2 r V_2(r) r^n$ are the moments of the twobody potential. Note that we obtain an expression similar to the above if we use an expansion of the form [21]

$$V_2(r) = \sum_{j=0} c_j b^{2j} \nabla^{2j} \delta^2(\vec{r}), \qquad (12)$$

where *b* is the range of the potential and c_j are related to the *j*th moment of the potential V_2 as $M_{2j} = 2^{2j} j! c_j b^{2j}$.

The spatial density is now determined by the variation $\delta(E - \mu N) = 0$, where μ is the chemical potential at zero temperature. The variation immediately gives the equation for the density

$$\frac{\pi\hbar^2}{m^*} \left[1 + \frac{m^*M_0}{2\pi\hbar^2} \right] \rho(r) + \frac{3\pi M_2}{8} \rho^2(r) + \frac{M_2}{4} \nabla^2 \rho(r) = \mu - V_1(r).$$
(13)

In the large-N limit we expect the density in the bulk to be approximately constant. We can therefore neglect the derivative term in this limit. Further, if the potential is extremely short ranged, the term proportional to the second moment of the potential may also be neglected. (We will elaborate on these approximations shortly.) Then the density is given by

$$\rho_0(r) = \begin{cases} \frac{m}{\pi \, \hbar^2 \alpha} \left[\mu - V_1(r) \right], & r \le r_0, \\ 0, & r > r_0, \end{cases}$$
(14)

where r_0 is the classical turning point defined by $\mu = V_1(r_0)$ and

$$\alpha = 1 + \frac{m^* M_0}{2\pi \hbar^2}$$
(15)

is now the statistics parameter as we show below. In the effective range expansion (12), $c_0 = M_0$. The expression for ρ_0 in Eq. (14) may be interpreted as if the fermions in the one-body confining potential V_1 are noninteracting, but that they obey the generalized exclusion statistics for occupancy at zero temperature,

$$n(\boldsymbol{\epsilon}) = \begin{cases} \frac{1}{\alpha}, & \boldsymbol{\epsilon} < \boldsymbol{\mu}, \\ 0, & \boldsymbol{\epsilon} > \boldsymbol{\mu}. \end{cases}$$
(16)

This may be easily seen as follows. For noninteracting fermions, the Thomas-Fermi density of states $g(\epsilon)$ in an external potential $V_1(r)$ is

$$g(\boldsymbol{\epsilon}) = 2 \int \frac{d^2 r \, d^2 p}{(2\pi\hbar)^2} \, \delta \bigg[\boldsymbol{\epsilon} - \frac{p^2}{2m^*} - V_1(r) \bigg]. \tag{17}$$

The overall factor of 2 on the right-hand side is due to the spin degeneracy. Using the new occupancies given by Eq. (16), we get

$$N = \frac{1}{\alpha} \int_{0}^{\mu} g(\epsilon) d\epsilon$$

= $\frac{1}{\alpha} \int 2 \frac{d^{2}r d^{2}p}{(2\pi\hbar)^{2}} \theta \bigg[\mu - \frac{p^{2}}{2m^{*}} - V_{1}(r) \bigg].$ (18)

The function $\theta(y) = 1$ for y > 0, and zero otherwise. Now performing the *p* integration immediately yields the total number of particles, with density $\rho_0(r)$ given by Eq. (14). Indeed we have now the precise condition under which ideal exclusion statistics is realized within the framework of the Thomas-Fermi method.

In the more realistic situation, the higher moments may not be neglected, and the system is a nonideal fractional statistics gas. In the thermodynamic limit, we may write

$$\rho(r) = \rho_0(r) \bigg[1 - \frac{3m^* M_2}{8\hbar^2 \alpha} \rho_0(r) + \cdots \bigg], \qquad (19)$$

where $\rho_0(r)$, given by Eq. (14), is the density for the ideal field emission spectroscopy case. Note that $M_2 = 4c_1b^2$ where *b* is the range of the potential. The typical densities in two dimensional systems of interest is of the order of $10^{-5}/\text{Å}^2$. Using the values of $m^* = 0.067m_e$, which is the effective electron mass in GaAs materials, and $\alpha \ge 1$

(but not very large), it is easy to estimate that the second term becomes important only for ranges of the order of 100 Å or above. Another way to view the problem is to regard the short-range part of the two-body interaction, which dominates M_0 , to alter the statistics only. The longrange part of V_2 , giving the higher moments, modifies the self-consistent mean field. Consider, for example, the electrons in two dimensional quantum dots. The two-body potential is usually taken to be the Coulomb interaction, and the confining potential of the device is modeled by the oscillator potential. However, it is expected that the effective two-body interaction after averaging over the probability densities in the direction perpendicular to the plane will be more complicated. Many qualitative features of the system may be explained by several choices of the potential. As in the case of FQHE liquids, we assume that the model interaction has a short-range part $V_{2s}(r)$ and a long-range part $V_{2l}(r)$. We use the moments expansion for the shortrange part and neglect the effect of higher moments. The self-consistent equation for the density is then given by

$$\rho(r) = \begin{cases} \frac{m^*}{\pi \hbar^2 \alpha} [\mu - U(r)], & r \le r_0, \\ 0, & r > r_0, \end{cases}$$
(20)

where the mean TF potential is defined as

$$U(r) = V_1(r) + \int d^2 r \,\rho(r') V_{2l}(|\vec{r} - \vec{r}'|). \quad (21)$$

The equation further simplifies for circularly symmetric density. Expanding the potential in partial waves,

$$V_{2l}(|\vec{r} - \vec{r}'|) = \frac{1}{\pi} \sum_{m=0}^{\infty} v_m(r, r') \cos(\theta - \theta'),$$

the TF potential reduces to

$$U(r) = V_1(r) + \int r' dr' \rho(r') v_0(r, r').$$
 (22)

In the above equation we have ignored the exchange effects that are not important for the long-range potentials. Thus Eq. (22) is the self-consistency condition to determine the density $\rho(r)$, and in general is not solvable analytically.

Finally we consider briefly the finite temperature problem using the Thomas-Fermi method. We restrict our attention to the case where the two-body potential is extremely short ranged and regard the system as ideal. The temperature T is expressed in units of the Boltzmann constant, so that it has the dimensions of energy. The onebody potential is now temperature dependent, and is given by

$$V(r,T) = V_1(r) + \frac{M_0}{2}\rho(r,T)$$

= $V_1(r) - (1 - \alpha)\frac{\pi\hbar^2}{m^*}\rho(r,T)$, (23)

where α is the statistics parameter defined by Eq. (15). We have assumed that the external potential $V_1(r)$ is temperature independent. In the above equation, the density $\rho(r, T)$ for the fermions is obtained from the relation (including the spin degeneracy of 2)

$$\rho(r,T) = \frac{2}{(2\pi\hbar)^2} \times \int \frac{d^2p}{\exp[(p^2/2m^* + V - \mu)/T] + 1},$$
(24)

and the chemical potential is determined by $N = \int d^2r \rho(r,T)$. The *p* integration above may be done analytically, giving

$$\rho(r,T) = \frac{m^*T}{\pi\hbar^2} \ln\{1 + \exp[-(V-\mu)/T]\}.$$
 (25)

This is inverted to give

$$\frac{\mu}{T} = \left[V + \frac{\pi\hbar^2}{m^*} \rho \right] / T + \ln[1 - \exp(-\pi\hbar^2\rho/m^*T)].$$
(26)

Substituting for *V* above from Eq. (23), we get

$$\frac{\mu}{T} = \left[V_1(r) + \alpha \, \frac{\pi \hbar^2}{m^*} \, \rho(r, T) \right] \Big/ T \\ + \ln[1 - \exp(-\pi \hbar^2 \rho / m^* T)]. \quad (27)$$

For a gas in the thermodynamic limit, we set $V_1(r) = 0$ above. Further, the spatial density ρ may be expressed as $2\rho_0$, where ρ_0 is the density for spinless particles. Then Eq. (27) reduces to the form

$$\frac{\mu}{T} = \alpha \, \frac{2\pi\hbar^2}{m^*T} \, \rho_0 \, + \, \ln[1 - \exp(-2\pi\hbar^2\rho_0/m^*T)].$$
(28)

Note that this is precisely the equation derived by Wu [7] [see his Eq. (23)] for a two dimensional gas obeying the statistics

$$n(\boldsymbol{\epsilon}) = \frac{1}{w[\exp(\boldsymbol{\epsilon} - \boldsymbol{\mu})/T] + \alpha}, \qquad (29)$$

with w(x) satisfying the functional equation

$$w^{\alpha}(1+w)^{1-\alpha} = x = \exp(\epsilon - \alpha)/T.$$
 (30)

Here, as in our case, $\alpha = 1$ corresponds to free fermions.

We have thus shown that in the large-N limit, ideal exclusion statistics may be realized in a system of spinhalf fermions with very short-range interactions. Note that this situation is peculiar to two dimensions since both the leading term in the moments expansion and the kinetic energy density have the same dependence on the spatial density.

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