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A description of semi-degenerate bound states of fermions

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Abstract. A trapezoidal approximation to the Fermi-Dirac distribution function is used in order to obtain a simple description of semi-degenerate bound-states of fermions. Our model coincides with the exact result up to the first correction in the low-temperature expansion while leading to finite equilibrium configurations; thus, it represents an alternative to the use of confining cells or of energy—or density—cutoffs. The atom and the self-gravitating cluster are worked out as explicit examples.

1. Introduction

As is well known, if the particles constituting a bound assembly satisfy a perfect-gas distribution function at non-zero constant temperature, then the high-energy tail of this distribution leads to an inconsistency when defining a finite number of particles in the assembly; this, physically, can be traced to the leakage induced by evaporation. (Of course, this does not take place when the bound state is spatially confined as, for example, in the case of the Wigner–Seitz cell used for atomic systems [1] to describe the equation of state (EOS) of matter at finite temperature and pressure.) There are, however, other physical entities where the concept of temperature is quite useful but where one would like to get rid of this inconsistency. Examples in this direction are some intrinsically-isolated low temperature fermionic clusters such as excited atomic nuclei or certain cold astrophysics bodies like white dwarfs or neutron stars. It is worth mentioning that the influence of the high energy tail is not just a technical nuisance. In the self-gravitating sphere of fermions, for example, the use of the Fermi–Dirac distribution function (FDDF) leads, at the periphery, to a density profile which decays proportionally to $1/r^2$, i.e. to an undesired unlimited value for the radius and total mass of this configuration [2]. For a good reference illustrating this point the reader may see [3]. The standard procedure for dealing with this problem consists of using a density cutoff in the resulting density profile or an energy cutoff in the energy distribution used as input [4, 5]. In this paper we present a simple alternative, applicable to the description of semi-degenerate bound states of fermions, which consists of approximating the FDDF by a trapezoidal model which is conveniently tailored so as to coincide with the FDDF up to the first leading correction in the low-temperature expansion of the thermodynamic magnitudes. As this model limits the momentum spectrum, it allows a consistent treatment of finite bound states; furthermore, its functional simplicity leads to a quite transparent description of these systems. We will

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start the discussion by fixing some points of our statistical-mechanics model and later we will analyse two paradigmatic applications.

Our basic hypothesis consists of replacing the standard FDDF

$$\mathcal{F}(\varepsilon)=\left[\exp\left(\frac{\varepsilon-\mu}{KT}\right)+1\right]^{-1}$$

by a trapezoidal approximation, $\mathcal{G}(\varepsilon)$, namely

$$\mathcal{G}(\varepsilon)=\begin{cases}1 & 0\leqslant\varepsilon\leqslant\mu-1/2\beta' \\ \frac{1}{2}-\beta'(\varepsilon-\mu) & \mu-1/2\beta'\leqslant\varepsilon\leqslant\mu+1/2\beta' \\ 0 & \varepsilon\geqslant\mu+1/2\beta'.\end{cases} \tag{1}$$

Here μ stands, just as in $\mathcal{F}(\varepsilon)$, for the chemical potential in the absence of external field and β', which is minus the trapezoidal slope, is proportional to the inverse of the temperature and will be fixed below. The particle density derived from (1) adopts the form

$$n=\frac{g\beta'}{15\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\times\begin{cases}[\mu+1/2\beta']^{5/2}-[\mu-1/2\beta']^{5/2} & \mu>1/2\beta' \\ [\mu+1/2\beta']^{5/2} & -1/2\beta'\leqslant\mu\leqslant1/2\beta' \\ 0 & \mu<-1/2\beta'\end{cases} \tag{2}$$

g being the degeneracy parameter and m the individual particle mass. For any T, $\mathcal{G}(\varepsilon)$ leads to the familiar relation $PV=\frac{2}{3}E$, and that with the identification $\beta'=(2\pi KT)^{-1}$ the expansion of n around its $T=0$ value coincides in the two first terms, i.e. those in T^0 and in T^2, with that derived from $\mathcal{F}(\varepsilon)$. This will be the value adopted for β' throughout the paper, and its use ensures that at low temperature the use of $\mathcal{F}(\varepsilon)$ or $\mathcal{G}(\varepsilon)$ is quantitatively equivalent.

Another interesting consequence of $\mathcal{G}(\varepsilon)$ is that at high $T(-1/2\beta'\leqslant\mu\leqslant1/2\beta')$, the EOS of this system adopts a simple polytropic form, with index equal to $\frac{5}{2}$,

$$P=\kappa n^{7/5}\qquad \kappa=\frac{2}{7}\left(\frac{15}{4}\right)^{2/5}\left[\frac{8\pi^3\hbar^3KT}{g(2m)^{3/2}}\right]^{2/5}. \tag{3}$$

This behaviour, which holds at the periphery of the bound states of particles no matter how small KT may be with respect to the Fermi energy (ε_F) at the centre, is ultimately responsible for closing the systems and avoiding the above-mentioned inconsistency induced by the use of the FDDF. Notice that at the edge of the bound states the effect of the trapezoidal truncation is that the classical gas EOS, $P\propto nT$, is replaced by equation (3).

Let us now build the structure of the atom and the self-gravitating fermionic sphere which derive from $\mathcal{G}(\varepsilon)$. As mentioned, they will be finite, and at the points of effective low-temperature ($KT\ll\varepsilon_F$), the resulting density coincides with that which would come from FDDF. These two applications will be worked out within a unified formalism: the statistical—or Thomas-Fermi (TF)—model.

2. The atom

By substituting (2) into Poisson's equation $\nabla^2\phi=4\pi en$, assuming $g=2$, and with the

change of variables:

$$C=\mu-e\phi \qquad \mu+\frac{1}{2\beta'}=\frac{Ze^2\chi}{r}$$
$$r=bx \qquad b=\left(\frac{9\pi^2}{128}\right)^{1/3}\frac{\hbar^2}{me^2Z^{1/3}} \tag{4}$$

where Z is the nuclear charge, one obtains

$$(-1)^p\ddot{\chi}=\frac{\chi^{3/2}}{x^{1/2}}\cdot\begin{cases}2\chi/5\alpha x[1-(1-\alpha(x/\chi))^{5/2}] & \chi/x>\alpha \\ 2\chi/5\alpha x & 0\leqslant\chi/x\leqslant\alpha \\ 0 & \chi<0\end{cases} \tag{5}$$

with $\alpha=2\pi KTbZ^{-1}e^{-2}$, $p=0$ and C being the generalized chemical potential. Equation (5) is, in our formalism, the finite-temperature version of the habitual TF equation in atomic physics, and tends to it at zero temperature. The effect of increasing T is included in the dimensionless parameter α; thus, as we see, the universality of TF at $T=0$ is only partially lost. We have assumed, as usual, that the nucleus is pointlike, thus the right-hand side of Poisson's equation is valid for all values of r except $r=0$. Therefore we will solve (5) subject to the basic condition $\phi(r)\to Ze/r$ as $r\to 0$, i.e. $\chi(x=0)=1$. Furthermore, neutral atoms satisfy the restriction $X\cdot\dot{\chi}(X)=0$, X being the atomic radius measured in b units. Thus, as in the $T=0$ case, the solution corresponding to the neutral case is asymptotic to the x axis. One can easily show that it fulfils $\chi\to(\frac{10}{9})^{2/3}\alpha^{2/3}/x^{1/3}$ when $x\to\infty$. The total energy of a neutral atom is

$$U=-\frac{Z^2e^2}{4b}\left[-2\dot{\chi}(x=0)-\int\dot{\chi}^2\,dx\right]. \tag{6}$$

As α departs from 0, the physical solutions of (5) differ from the case $T=0$ (see figure 1). Table 1 (third column) contains several values of U. For very small α, the equation

$$\frac{U-U(\alpha=0)}{Ze^2/b}=1.345\alpha^2 \tag{7}$$

is a good fit for U and describes the initial increase of energy with temperature in this system.

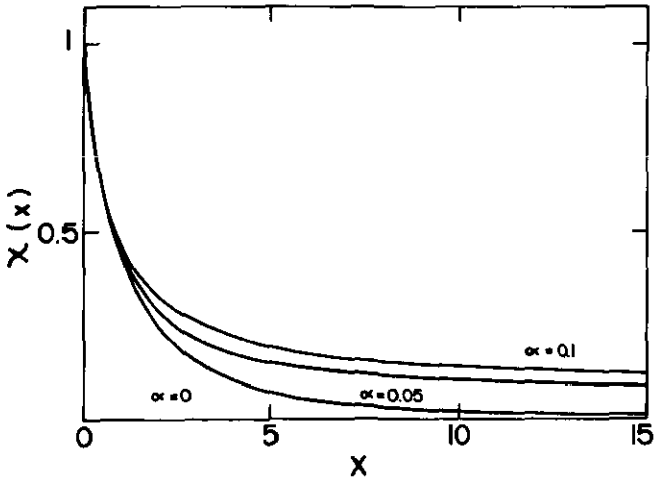

Figure 1. Physical solutions of (5) in the atomic case.

Table 1. Total energy as a function of α.

α	$U\Big/\frac{GM^2}{b}$	$U\Big/\frac{Z^2e^2}{b}$
0	−0.08409	−0.6806
0.01	−0.08403	−0.6803
0.03	−0.08350	−0.6794
0.05	−0.08245	−0.6782
0.10	−0.07704	−0.6745

3. Self-gravitating cluster

Now we study the structure formed by N non-relativistic fermions of mass m, linked together by their own gravity [6]. Inserting (2), with $\rho = mn$, into the Newtonian equation of gravity $\nabla^2\phi = 4\pi G\rho$, again with $g = 2$, and with the change of variables [3]

$$C = \mu + m\phi \qquad \mu + \frac{1}{2\beta'} = \frac{GMm\chi}{r}$$
$$r = bx \qquad b = \left(\frac{9\pi^2}{128}\right)^{1/3} \frac{\hbar^2}{Gm^3N^{1/3}} \tag{8}$$

($R = bX$ and $M = Nm$ being the radius of the cluster and total mass respectively), we again obtain equation (5) but with $p = 1$. In this case $\alpha = 2\pi KTbG^{-1}m^{-2}N^{-1}$. Thus, apart from the minus sign induced by p which reflects the attraction between the particles, the parallelism with the atomic case is absolute. Note that in these new dimensionless variables N, the number of particles of the cluster, appears [7] at the same position as Z, i.e. the nuclear charge of the atom. Here, for any α, the physical solutions depart from zero, $\chi(x = 0) = 0$, and self-consistency in the total mass imposes the restriction $X \cdot \dot{\chi}(X) = -1$. Various physical solutions of (5) are plotted in figure 2.

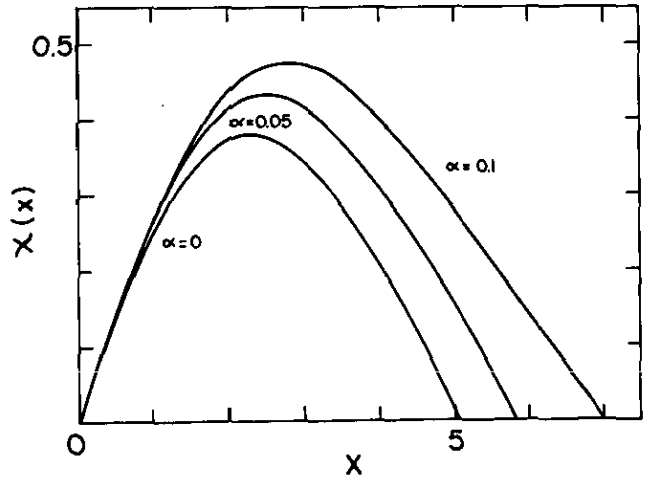

Figure 2. Physical solutions of (5) in the case of self-gravitating clusters.

The total energy of the cluster is

$$U = -\frac{GM^2}{4b}\left[\frac{1}{X} + \int \dot{\chi}^2 \, dx\right]. \tag{9}$$

Table 1 (second column) shows several values of U. In the same spirit of (7), here the excitation energy measured in GM^2/b units adopts the form $0.651\alpha^2$.

Since at $T = 0$ the structure of the self-gravitating cluster of fermions is that of a pure $n = \frac{3}{2}$ polytrope [6], we observe that in our framework, at low-temperature the structure of these configurations evolves from the approximate $n = \frac{3}{2}$ polytropic nature in the interior (where $KT \ll \varepsilon_F$), to the above-mentioned $n = \frac{5}{2}$ behaviour at the edge. This contrast with the result obtained when the FDDF is used. In this case one starts from $n = \frac{3}{2}$ at the centre and ends with $n = \infty$ (the classical perfect gas) at the border. Thus, we see how the trapezoidal approximation induces an effective cutoff in the polytropic index of the resulting structure of the cluster.

4. Conclusions

In our opinion, the method presented here constitutes an elegant alternative for the description of finite bound-states of fermions at low temperatures. The trapezoidal approximation to the FDDF is extremely simple and provides a natural cutoff for the individual particle energy which makes it unnecessary to use the habitual more-or-less justified cutoffs. In our model, for the atom and for the self-gravitating cluster, the departure from the $T = 0$ case is controlled solely by a dimensionless parameter α, which is proportional to the ratio between the thermal energy and the TF ground-state energy. In subsequent work we will develop the applications outlined here. In the field of atomic physics, for example, one of the appealing areas for testing this method is the physics of small metal clusters [8] because they are produced isolated and at non-zero temperature. It is appropriate to remark that here the trapezoidal approximation has been plugged into the TF model [9]; analogously it may be used in the Hartree-Fock [10] or Kohn-Sham formalisms, to describe finite-temperature systems from a microscopic point of view [11].

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