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***Research Article***

# QUANTUM HARD-SPHERE ASSEMBLY OF FERMIONS

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**ABSTRACT**
The thermodynamic properties of a hard-sphere assembly of fermions in which the $^3He$ atoms are assumed to be interacting via a hard-sphere interaction has been calculated. The variation of energy per particle $\left(E/N\right)$ with temperature $T$ is non-linear due to the thermal factor, but becomes insignificantly minimal at low temperatures below 4 K due to zero-point effects becoming visible. The specific heat $C_v$ increases with increase in temperature to a point of inflection at a transition temperature $T_c$ = 18.67 K and this value closely compares well with $T_c$ = 20.3 K calculated using the Fermi energy formulation. This result indicates that, a hard-sphere Fermi gas of $^3He$ will undergo a phase transition at $T_c$ = 18.67 K.

***Keywords:*** *Thermal Factor, Fermions, Transition Temperature*

## INTRODUCTION

Fermions have half-integral spin and constitute the second half of the particles family. To tell whether an atom is a fermion we look at the total number of protons, neutrons, and electrons making up that atom. Since these are all spin $1/2$ fermions adding up an odd number of them will make an atom a fermion (half integer spin). Fermions obey the Pauli Exclusion Principle. This means that two indistinguishable fermions can never occupy the same quantum state.

Instead, in the limit of absolute zero temperature they fill the lowest energy states with exactly one atom per state in an arrangement known as the Fermi sea.

All energy states up to the Fermi energy $E_F$ are filled with particles in two different spin states. Such a Fermi sea is not superfluid and the assembly of fermions will be effectively a non-interacting system of particles. Fermi gas forms a useful first approximation in the theory of metals, in the theory of $^3He$, in studies of nuclear structure, nuclear matter and neutron stars.

To understand the behavior of such many-body assemblies composed of fermions, some interaction must be included between the particles. In this manuscript it is assumed that the interaction between two fermions in the system is a hard-sphere interaction.

It should also be understood that in the long wavelength limit only s-wave scattering is considered, and for hard-sphere gas the scattering length 'a' is just the hard-sphere diameter (Beliaev, 1958).

A hard-sphere system of fermions with density ranging from very low to very high will be considered to obtain an expression for the energy per particle $\left(E/N\right)$. For fermions, we need to satisfy Pauli exclusion principle which leads to repulsion between fermions when they try to approach each other to occupy the same energy state.

A gas or liquid composed of $^3He$ is a well known assembly of fermions in which particles can be assumed to interact via the pairwise potential (Aziz *et al*., 1979), and the energy of such a system can be calculated. Neutron matter and nuclear matter are other systems of fermions.

For an N-identical fermion system, the energy $E$ is given by (Baker, 1971) for a low-density system,

$$\frac{E}{N}=\frac{3}{5}\frac{\hbar\kappa_F^2}{2m}\left\{\begin{array}{l}1+C_1(\kappa_F a)+C_2(\kappa_F a)^2+\left[\frac{C_3 r_0}{2a}+\frac{C_4 A_1(0)}{a^3}+C_5\right](\kappa_F a)^3\\ +C_6(\kappa_F a)^4 \ell og(\kappa_F a)+\left[\frac{C_7 r_0}{2a}+C_8\frac{A_0^{''}}{a^3}+C_9\right](\kappa_F a)^4+0(\kappa_F a)^4\end{array}\right\} \quad 1$$

where the (Baker *et al*., 1982) $C_j$'s $(j=1,2,.....9)$, for $v=2$ and $v=4$, are dimensionless co-efficients depending on $v$, which is the number of intrinsic degrees of freedom of each fermion. For instance, for $v=4$, $C_2=0.556610$ and $C_9$ is not available for $v=4$. The Fermi-momentum $\hbar\kappa_F$ in terms of the fermion number density $\rho$ is given by,

$$\rho=\frac{N}{V}=\frac{v\kappa_F^3}{6\pi} \quad 2$$

where, $V$ is the volume of the system. The quantities $a$, $r_0$ and $A_1(0)$ are parameters containing information related to two-body scattering due to a central potential $U(r)$. Whereas, $A_0^{''}(0)$ cannot be related to the scattering phase shift alone, but is potential-shape dependent and can thus be interpreted as the first correction to the static limit, while $C_9$ has a three-body cluster contribution.

In fact, the low density expansion given in Eqn (1) breaks down at moderate and high densities including the saturation liquid density of $^3He$ and nuclear matter.

For fermion hard-sphere system Eqn (1) can be re-written as,

$$\frac{E}{N}=\frac{3}{5}\frac{\hbar^2\kappa_F^2}{2m}e_0(x) \quad 3$$

Where $x=\kappa_F\chi_0$ and $\chi_0$ is the hard-core diameter. Now $e_0(x)$ can be written as,

$$e_0(x)\cong 1+C_1x+C_2x^2+\left(\frac{C_3}{3}+\frac{C_4}{3}+C_5\right)x^3+C_6x^4\ell ogx+\left(\frac{C_7}{3}-\frac{C_8}{3}+C_9\right)x^4+0(x^4) \quad 4$$

For $v=2$, the value of (Baker, 1971; Baker *et al*., 1982) $C_6=0$ and Eqn (4) simplifies to,

$$e_0(x)\cong 1+D_1x+D_2x^2+D_3x^3+D_4x^4+0(x^4) \quad 5$$

for $x<<1$, with the *D*'s expressible in terms of the *C*'s. The ultimate aim is to calculate the value of $E/N$ for very high densities when the system of hard-spheres of fermions will go to close packing (*cp*); it does not matter whether the packing is random or regular. But it should be understood that the regular *cp* will be face-centered-cubic, *fcc*, or hexagonal-close-packing, *hcp*.

***Theory***

Ultimately, the value of $E/N$ has to be calculated from Eqn (3). This requires that the function $e_0(x)$ should not have a zero in its denominator since that will make the energy diverge. We have to work in the region of physical interest, and that is the one in which $0\le x\le 3.47$, and in this region the energy does not diverge at any close packing. However, the value of $e_0(x)$ will be approximated as (Solis *et al*., 2008),

$$e_0(x)\cong 1+C_1x+C_2x^2+\left(\frac{C_3}{3}+\frac{C_4}{3}+C_5\right)x^3 \quad 6$$

For [4] $v=2$ (two degrees of freedom for the fermions), $C_1=0.353; C_2=0.185; C_3=0.384$

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Here $x = \kappa_F \chi_0$ where $\chi_0$= 2.1117 is the hard-core diameter for $^3He$. Similarly, [5] for $v = 4$ (four degrees of freedom) $C_1 = 1.0610; C_2 = 0.5566; C_3 = 1.3006.$

The general expression for $\kappa_F$ via the Fermi energy $\in_F$ (Khanna, 1986) is given by,

$$\in_F = \frac{\kappa_F^2 \hbar^2}{2m} = \left(\frac{h^2}{8m}\right)\left(\frac{3}{\pi}\rho\right)^{\frac{2}{3}} \qquad 7$$

or

$$\kappa_F = \left(3\pi^2 \rho\right)^{\frac{1}{3}} \qquad 8$$

Where in our case the mass *m* is for $^3He$ atom, and $\rho = 0.86\rho_0$. But for *cp* or *hcp*, $\rho$ in Eqn (8) may be replaced by $\rho_0 = \sqrt{2}/\chi_0^3$ where the assembly may have reached the crystalline state.

For *hpc* or *fcc*, the value of $E/N$ is given by (Rhen and Llano, 1989),

$$\frac{E}{N} = Q_v \rho^{\frac{2}{3}} + \left(\frac{v-1}{v}\right)\frac{2\pi\hbar^2 \chi_0}{m}\left[\frac{1}{\left(\rho^{-\frac{1}{3}} - \rho_0^{-\frac{1}{3}}\right)\left(\rho^{-\frac{1}{3}} + b(v)\rho_0^{-\frac{1}{3}}\right)}\right] \qquad 10$$

Where

$$Q_v = \frac{3\hbar^2}{10m}\left(\frac{6\pi^2}{v}\right)^{\frac{2}{3}} \qquad 11$$

and

$$b(v) = \left[\left(\frac{v-1}{v}\right)(b+1) - 1\right] \approx b \qquad for\, v \to \infty \qquad 12$$

With $v = N \to \infty$, in the low density limit,

$$\frac{E}{N}\underset{\rho \to 0}{=} Q_v \rho^{\frac{2}{3}} + \left(\frac{v-1}{v}\right)\frac{2\pi\hbar^2 \rho \chi_0}{m} \qquad 13$$

Another expression for energy per particle that has been used for $^3He$ is given in Eqn (3) (Panoff, 1990; Panoff and Carlson, 1989).

The value of the total energy *E* can be obtained from Eqn (13) since all the parameters in Eqn (13) are known. In the limit of small $\rho$ ($\rho \to 0$), let *E* be represented by $E_0$. To understand the temperature dependence of the energy *E*, specific heat $C_v$, entropy *S* and the transition temperature $T_c$; $E_0$ will be multiplied by the thermal activation factor $\boldsymbol{\tau}$, such that,

$$\tau = \exp\left(-\frac{E_0}{\kappa_B T}\right) \qquad 14$$

where $k_B$ is the Boltzmann constant.

And the total energy *E* may be written as,

$$E = E_0 \exp\left( -\frac{E_0}{\kappa_B T} \right) \qquad 15$$

The specific heat $C_v$ becomes,

$$C_v = \frac{\partial E}{\partial T} = \frac{E_0^2}{\kappa_B T^2} \exp\left( -\frac{E_0}{\kappa_B T} \right) \qquad 16$$

The entropy $S$ becomes,

$$S = \int \frac{C_v dT}{T} = \int \frac{E_0^2}{\kappa_B T^3} \exp\left( -\frac{E_0}{\kappa_B T} \right) dT \qquad 17$$

or

$$S = \kappa_B \left( \frac{E_0}{\kappa_B T} + 1 \right) \exp\left( -\frac{E_0}{\kappa_B T} \right)$$

18

The transition temperature $T_c$ will be given by,

$$\left( \frac{\partial C_v}{\partial \mathrm{T}} \right)_{T=T_c} = 0 = \frac{E_0^2}{\kappa_B T^2} \left( -\frac{E_0}{\kappa_B} \right) \left( -\frac{1}{T^2} \right) \exp - \frac{E_0}{\kappa_B T} + \left( \frac{2E_0^2}{\kappa_B T^3} \right) \exp\left( -\frac{E_0}{\kappa_B T} \right) \qquad 19$$

For $T = T_c$ in Eqn (19), we get,

$$T_c = \frac{E_0}{2\kappa_B} = 18.67K \qquad 21$$

$T_c$ will be the temperature at which phase transition can take place in a system of hard-sphere gas of fermions ($^3He$).

***Calculations***

To do calculations for a system composed of $^3He$ atoms, $v$ =2, $Q_v$ is given by Eqn (11), $\rho = 0.86\frac{\sqrt{2}}{\chi_0^3}$ but $\chi_0$ = 2.1117Å, and assuming $N$ to be the number of particles in the unit volume, then $N = \rho$.
The mass of $^3He$ atom $m$ = 3.0160293 x$10^{-24}$g,
Eqn (13) will be used to get the value of $E_0$ and Eqn (15) for $E$. Specific heat $C_v$ will be calculated from Eqn (16), entropy $S$ from Eqn (18) and the transition temperature $T_c$ using Eqn (21).

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**RESULTS AND DISCUSSION**

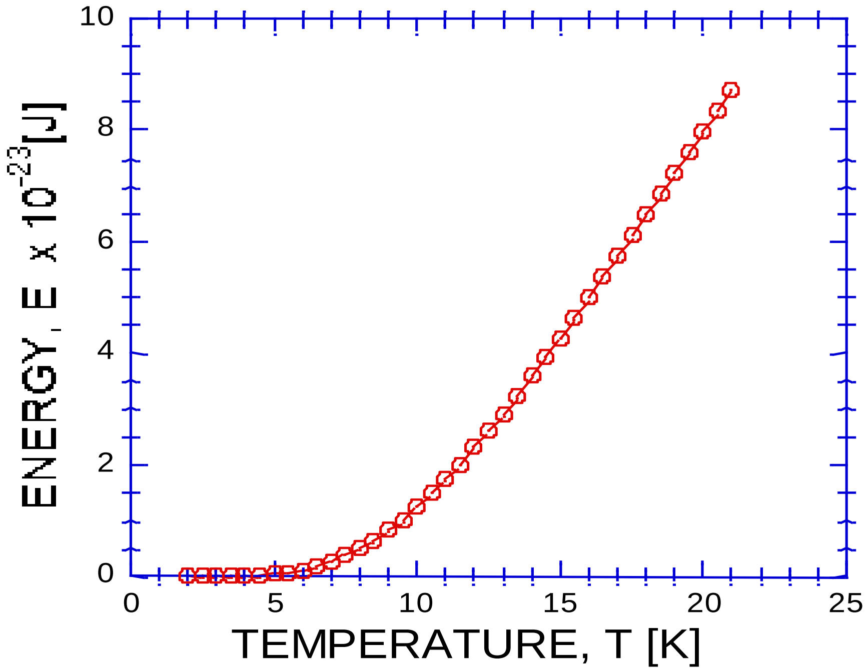


**Figure 1: Energy variation with Temperature**

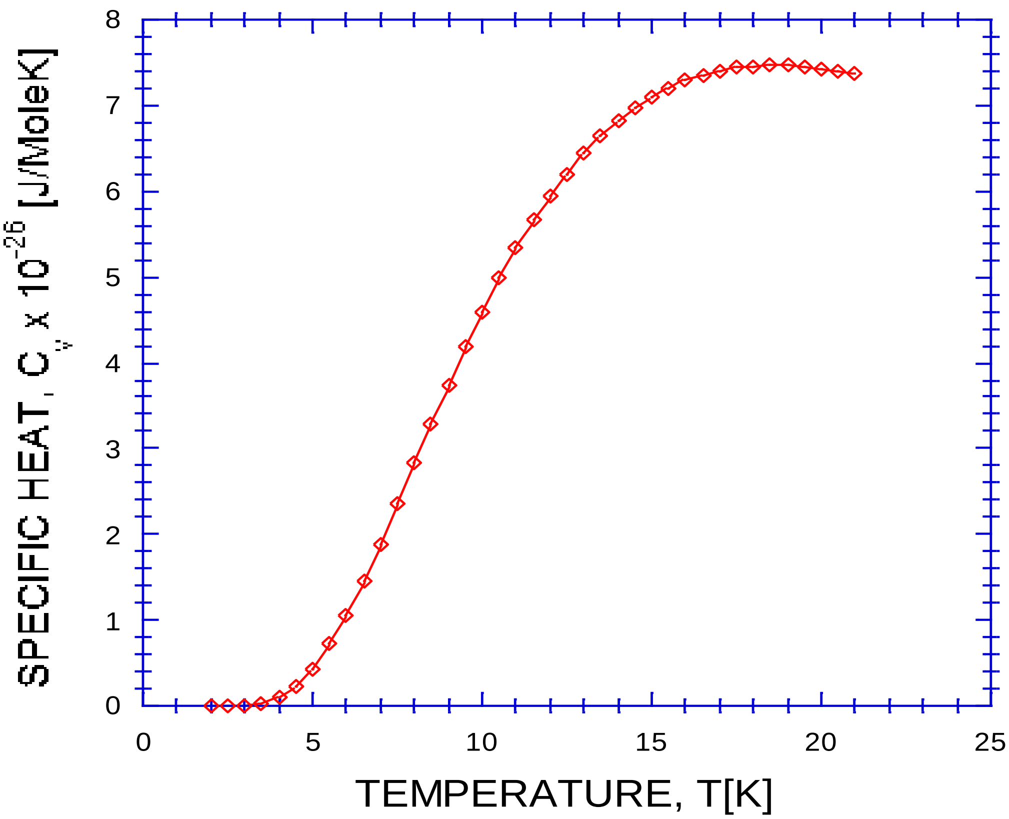


**Figure 2: Specific Heat variation with Temperature**

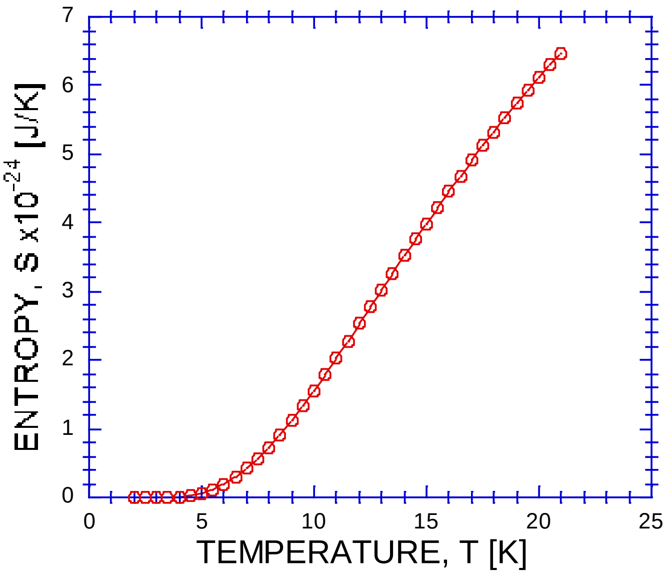


**Figure 3: Entropy variation with Temperature**

The calculations done for *E*, $C_v$ and *S* are plotted in Figure 1, Figure 2 and Figure 3 respectively. Figure 1 shows that the energy *E* of the system increases as *T* increases, and this is what it should be thermodynamically. Figure 2 shows the variation of $C_v$ with *T*, and as *T* increases, the value of $C_v$ shows a point of inflection at a temperature $T_c$ called the critical or transition temperature, and the value of $T_c$ = 18.67 K. According to this calculation, a gas of $^3He$ will undergo a phase transition at $T_c$ = 18.67 K provided the $^3He$ atoms are assumed to be interacting via a hard-sphere interaction. Such an interaction is characterized by the s-wave scattering length "a" (hard-core diameter = $\chi_0$). Mean-field theory gives a relation (Holland *et al*., 2001; Leggett, 1980; Heiselberg, 2000) between $T_c$ and the Fermi temperature $T_F$ such that,

$$\frac{T_c}{T_F} \approx \exp\left(-\frac{\pi}{2|\chi_0|\kappa_F}\right) \qquad 19$$

The Fermi temperature for fermions is,

$$T_F = \frac{\hbar^2}{2m\kappa}\left(3\pi^2\rho\right)^{\frac{2}{3}} \qquad 20$$

Where the momentum vector, $\kappa_F = \left(3\pi^2\rho\right)^{\frac{1}{3}}$, and giving the value $|\chi_0|\kappa_F = 3.30$. Since for the $^3He$ hard-sphere gas, the values of $|\chi_0|\kappa_F$ may lie between 0 and 3.47, in Eqn (19) using $|\chi_0|\kappa_F = 3.30$, the value of $T_c$ = 20.3 K. This transition temperature closely compares with our calculated value of 18.67K. The variation of $C_v$ with *T* in Fig. 2 qualitatively agrees with the variation of $C_v$ with *T* (Mishra and Ramakrishnan, 1985).

Our calculations lead to the conclusion that an assembly of hard-sphere $^3He$ can undergo a phase transition at a transition temperature $T_c$ = 18.67 K.

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