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Research Article

INTERNAL ENERGY OF A GRAND CANONICAL ENSEMBLE OF A MIXTURE OF HELIUM ISOTOPES WITH DUO-FERMION SPIN DEGENERACY

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ABSTRACT
We have considered a system consisting of a mixture of helium isotopes ^{3}He-^{4}He interacting weakly in pairs. The partition function of the system with duo-spin and varying number of bosons and fermions is developed to bring out the superfluid properties of the system. The study focused on a Grand Canonical ensemble of ^{3}He - ^{4}He isotopes whose superfluid properties have been determined by distinctively singling out the duo spin component. The internal energy was established algebraically, analyzed and found out to be increasing with temperature. For high temperatures, internal energy remains constant due to particle saturation.

***Keywords**: Grand Canonical Ensemble, super fluid, Duo Spin Component*

INTRODUCTION

Statistical thermodynamics explains the thermodynamic behavior of macroscopic systems as derived from the properties of microscopic systems. The ensemble model approach consisting of large collection of particles can be used to study statistical mechanics. Bosons are atoms with even sum of the numbers of elementary particles, possessing integral spin angular momentum. They obey Bose-Einstein statistics. Fermions are atoms with an odd sum of the number of elementary particles; possess odd half-integral spin angular momentum. They obey Fermi-Dirac statistics

This study focuses on a system with varying number of particles. Thus particle occupancy is not solely dependent on temperature. These conditions apply to a grand canonical ensemble which may be applicable to real systems (Sakwa *et al.*, 2013)

The stable fermionic (^{3}He) and bosonic (^{4}He) isotopes of helium (in their ground state), as well as mixtures of the two, have exhibited quantum properties in both the liquid and solid phases (McNamara *et al*, 2013). More recently, the advent of laser cooling and trapping techniques lead to the production of Bose-Einstein condensates (BECs) and the observation of Fermi degeneracy in weakly interacting atomic gases. Bose condensed atomic species have each been exhibiting its own unique features. Studies of degenerate fermions have a similar impact, and they have been the object of much study in recent years, culminating in the detection of superfluidity across the entire crossover region between BEC and Bardeen-Cooper-Schrieffer pairs (Wu C *et al.*, 2011). Degenerate atomic Fermi gases have been difficult to realize for two reasons: first, evaporative cooling relies upon elastic re-thermalizing collisions, which at the temperatures of interest (<1 mK) are primarily *s*-wave in nature and are forbidden for identical fermions; and second, the number of fermionic isotopes suitable for laser cooling and trapping is small(Win Vassen,2013). Sympathetic cooling overcomes the limit to evaporative cooling by introducing a second component (spin state, isotope or element) to the gas; thermalization between the two components then allows the mixture as a whole to be cooled.

Rafael E et al(2015), studied the contact and static factor of bosonic and fermionic systems, they observed that few-body ensembles consist of majority atoms obeying certain statistics (Fermi or Bose) and an impurity atom in a different hyperfine state. The repulsive interactions between majority-impurity and majority-majority were varied from weak to strong. They showed that the majority-impurity repulsion was mainly responsible for the loss of coherence in the strongly interacting regime. The momentum distribution follows the C/p^4 universal behaviour for the high momentum tail, but the contact C is strongly dependent on the strength of the majority-impurity and in a different way on the majority-majority interactions. The static structure factor of the majority atoms exposes a low momentum peak for strong majority-impurity repulsion, which is attributed to an effective attraction not expected for purely repulsive forces..

The Partition function for a Grand canonical ensemble for a mixture of ^{3}He-^{4}He with duo spin has been developed. The results of key derivations and analysis of particle and internal energy are presented.

Theoretical Derivations

Introduction

To study the properties of a mixture of bosons and fermions with different concentrations, consider an assembly consisting of N particles with N_b being the number of bosons and N_f being the number of fermions.

Therefore, $N = N_b + N_f$ (1)

The energy states of the assembly are $\varepsilon_1, \varepsilon_2, \varepsilon_3, \ldots\ldots\ldots\ldots\ldots\ldots \varepsilon_{n.} \ldots..$ and in the statistical equilibrium, the number of particles or systems assigned to this energy levels are $n_1, n_2, n_3, \ldots\ldots\ldots\ldots\ldots\ldots n_j \ldots..$ respectively such that

$$\sum_{J=1}^{\infty} n_j = N \tag{2}$$

And

$$\sum_{j=1}^{\infty} n_j \varepsilon_j = E \tag{3}$$

Similarly for a jth energy level,

$$n_j = n_{jb} + n_{jf} \tag{4}$$

Where,

$n_{jb} =$ The number of bosons in the jth energy level

$n_{jf} =$ The number of fermions in the jth energy level

Let ω_j be the degeneracy of the jth level. Then the number of ways P_{jb} in which n_{jb} bosons can be assigned to ω_j states in the jth level is given by

$$P_{jb} = (\omega_j)^{n_{jb}} \tag{5}$$

However , the occupancy of fermions is subject to Pauli's exclusion principle. Then the number of ways P_{jf} in which n_{jf} fermions can be assigned to ω_j states in the jth level is given by

$$P_{jf} = \frac{\omega_j!}{n_{jf}!(\omega_j - n_{jf})!} \tag{6}$$

Fermion occupancy of any energy level is independent of bosons occupancy of that energy level i.e. $n_{jb} > n_{jf}$ hence the above probabilities are multiplicative. The combined number of ways of assigning n_{jb} bosons and n_{if} fermions in an energy level is given by

$$P_{jbf} = \frac{(2_j)^{n_{jb}}.(2_j)!}{n_{jf}!(2 - n_{jf})!(n_{jb} - n_{jf})!} \tag{7}$$

Where 2 is the spin degeneracy of a binary system of helium isotopes particles.

In the above expression, permutations among identical pairs are eliminated by dividing by $n_{jf}!$. Similarly, dividing by $(n_{jb} - n_{jf})!$, eliminates all identical complexions of unpaired bosons.
The total number of ways of distributing these particles among the independent energy levels (*j* = 1, 2, 3…) is the product of such expressions in equation (7).

$$C_{bf} = \prod_{j=1}^{\infty} P_{jbf} = \prod_{j=i}^{\infty} \left[\frac{(2_j)^{n_{jb}}.(2_j)!}{n_{jf}!(2-n_{jf})!(n_{jb}-n_{jf})!} \right] \tag{8}$$

The concern now is how these n_j particles distribute themselves in thermal equilibrium to occupy maximum volume in phase space. Thus, for maximum C_{bf}, we allow the variation of C_{bf} with respect to n_{jb} and n_{jf} set the result equal to zero. By use of the Stirlings' approximation and the Langrage undetermined multipliers, the most probable distribution in energy for bosons and fermions in the degenerate system is determined as
The total energy E of the assembly will be given by

$$E = E_b + E_f \tag{9}$$

Where E_b is the energy of the bosons and E_f is the energy of the fermions.
Simplifying equation (8) by using Stirling's approximations gives

$$\ln C_{bf} = \sum_{j=1}^{\infty} (n_{jb}+1)\ln 2! - [\ln n_{jf}! + \ln(2-n_{jf})! + \ln(n_{jb}-n_{jf})! \tag{10}$$

Expanding and then differentiating equation (10) with respect to n_{jf} gives

$$\frac{\partial}{\partial n_{jf}}(\ln C_{bf}) = \ln\left(\frac{(2-n_{jf})(n_{jb}-n_{jf})}{n_{jf}} \right) \tag{11}$$

Also, differentiating equation (10) with respect to n_{jb} gives

$$\frac{\partial}{\partial n_{jb}}(\ln C_{bf}) = \ln\left(\frac{2}{n_{jb}-n_{jf}} \right) \tag{12}$$

To maximize $\ln C_{bf}$, we differentiate $\ln C_{bf}$ and set the result to zero i.e.

$$\partial \ln C_{bf} = \sum_{j=1}^{\infty} \left[\frac{\partial}{\partial n_{jb}} (\ln C_{bf}) dn_{jb} \right] + \sum_{j=1}^{\infty} \left[\frac{\partial}{\partial n_{jf}} (\ln C_{bf}) dn_{jf} \right] = 0 \tag{13}$$

∂n_{jb} and ∂n_{jf} represent allowable changes in the distribution numbers from the required distribution, they should continue to satisfy the equation given by equation (1) to (4). Since N and E are fixed, the variation in n_{jb} and n_{jf} must satisfy the following equations.

$$\sum_{j=1}^{\infty} dn_{jb} + \sum_{j=1}^{\infty} dn_{jf} = 0 \tag{14}$$

$$\sum_{j=1}^{\infty} \varepsilon_j dn_{jb} + \sum_{j=1}^{\infty} \varepsilon_j dn_{jf} = 0 \tag{15}$$

Combine equations (13), (14) and (15) by Lagrange's undetermined multipliers denoted by α and β. Multiplying first and second terms of equation (14) by $-\alpha_b$ and $-\alpha_f$ respectively, equation (15) by $-\beta$ and adding to equation (13).

$$\sum_{j=1}^{\infty} -\alpha_b dn_{jb} + \sum_{j=1}^{\infty} \varepsilon_j dn_{jb} + \sum_{j=1}^{\infty} \frac{\partial}{\partial n_{jb}} \ln C_{bf} dn_{jb} = 0$$

Rearranging the above equation gives

$$\sum_{j=1}^{\infty} \left\{ \frac{\partial}{\partial n_{jb}} \left(\ln C_{bf} \right) - \left(\alpha_b + \beta \varepsilon_j \right) \right\} dn_{jb} = 0 \qquad (16)$$

Similarly, multiplying first and second terms of equation (14) by -α_b and -α_f respectively, equation (15) by -β and adding to equation (13).

$$\sum_{j=1}^{\infty} \left\{ \frac{\partial}{\partial n_{jf}} \left(\ln C_{bf} \right) - \left(\alpha_f + \beta \varepsilon_j \right) \right\} dn_{jf} = 0 \qquad (17)$$

The algebraic sum of equation (16*)* and (17) fields equation (18)

$$\sum_{j=1}^{\infty} \left\{ \frac{\partial}{\partial n_{jb}} \left(\ln C_{bf} \right) - \left(\alpha_f + \beta \varepsilon_j \right) \right\} dn_{jb} + \sum_{j=1}^{\infty} \left\{ \frac{\partial}{\partial n_{jf}} \left(\ln C_{bf} \right) - \left(\alpha_f + \beta \varepsilon_j \right) \right\} dn_{jf} = 0 \qquad (18)$$

In equation (18), we set the coefficients of dn_{jb} and dn_{jf} to zero since; dn_{jb} and dn_{jf} are allowable varriables thus the above equation can be written as

$$\frac{\partial}{\partial n_{jb}} (\ln C_{bf}) - (\alpha_b + \beta \varepsilon_j) = 0 \qquad (19)$$

$$\frac{\partial}{\partial n_{jf}} (\ln C_{bf}) - (\alpha_f + \beta \varepsilon_j) = 0 \qquad (20)$$

Substituting equation (12) in equation (19), we get

$$\ln \left(\frac{2}{n_{jb} - n_{jf}} \right) = \left(\alpha_b + \beta \varepsilon_j \right) \qquad (21)$$

$$\frac{2}{n_{jb} - n_{jf}} = \exp\left(\alpha_b + \beta \varepsilon_j \right) \qquad (22)$$

Making n_{jb} the subject in equation (22), yields

$$n_{jb} = \frac{2}{\exp\left(\alpha_b + \beta \varepsilon_j \right)} + n_{jf} \qquad (23)$$

Substituting for $\beta = \dfrac{1}{KT}$ and $\alpha_b = -\dfrac{\mu_b}{KT}$

$$n_{jb} = 2.\exp\left[\frac{\mu_b - \varepsilon_j}{KT} \right] + n_{jf} \qquad (24)$$

Similarly, substituting equation (11*)* into (20*)* and simplifying, we get

$$\ln \left(\frac{\left(2 - n_{jf} \right)\left(n_{jb} - n_{jf} \right)}{n_{jf}} \right) - \left(\alpha_b + \beta \varepsilon_j \right) = 0$$

$$n_{jf} = \frac{4}{2 + \exp\left(\alpha_f + \beta \varepsilon_j \right) \exp\left(\alpha_b + \beta \varepsilon_j \right)}$$

Substitute $\alpha_f = -\frac{\mu_f}{KT}, \beta = \frac{1}{KT}$ and $\alpha_b = -\frac{\mu_b}{KT}$ to obtain

$$n_{jf} = \frac{4}{2 + \exp\left[\frac{-\mu_f + \varepsilon_j - \mu_b + \varepsilon_j}{KT}\right]}$$

This simplifies to

$$n_{jf} = \frac{4}{2 + \exp\left[\frac{2\varepsilon_j - \mu_f - \mu_b}{KT}\right]} = \frac{2}{1 + \frac{1}{2}\exp\left[\frac{2\varepsilon_j - \mu_f - \mu_b}{KT}\right]} \tag{25}$$

Equation (25) gives the expression for the distribution particles for helium-3 particles which have a spin degeneracy of two.

Also, substitute for n_{jf} in equation (28), to obtain

$$n_{jb} = 2\left[\exp\left(\frac{\mu_b - \varepsilon_j}{KT}\right)\right] + n_{jf} = 2.\exp\left(\frac{\mu_b - \varepsilon_j}{KT}\right) + 4\left[2 + \exp\left(\frac{2\varepsilon_j - \mu_b - \mu_f}{KT}\right)\right]^{-1} \tag{26}$$

Equation (26) gives the most probable distribution particles for bosons (Helium-4) in the mixture. Where T is the temperature, K is the Boltzmann constant, μ_f is the chemical potential of the fermions and μ_b is the chemical potential of the bosons.

Combining equation (25) and (26) gives

$$n_{jbf} = 8\left[2 + \exp\left(\frac{2\varepsilon_j - \mu_b - \mu_f}{KT}\right)\right]^{-1} + 2.\exp\left(\frac{\mu_b - \mu_f}{KT}\right) \tag{27}$$

Equation (27) gives an expression for the most probable distribution for a mixture of bosons and fermions with duo-spin degeneracy of two.

Partition Function

The partition function of a grand canonical ensemble where both N_b and N_f are variable can be derived from

$$Z(\mu_b, \mu_f, V, T) = \sum_{N_b, N_f}^{\infty} \exp\left(\frac{-\xi}{KT}\right).\exp\left[\frac{(\mu_b N_b + \mu_f N_f)}{KT}\right]$$

$$Z(\mu_b, \mu_f, V, T) = \sum_{N_b, N_f}^{\infty} \left\{8\left[2 + \exp\left(\frac{2\varepsilon_j - \mu_b - \mu_f}{KT}\right)\right]^{-1} + 2.\exp\left(\frac{\mu_b - \varepsilon_f}{KT}\right)\right\}\exp\left(\frac{-\xi + \mu_b N_b + \mu_f N_f}{KT}\right)$$

This simplifies to

$$Z(\mu_b, \mu_f, V, T) = \sum_{N_b, N_f}^{\infty} \left\{2\left[4 + 2\exp\left(\frac{\mu_b - \mu_f}{KT}\right) + \exp\left[2\left(\frac{-\mu_f + \varepsilon_j}{KT}\right)\right]\right]\right\} \frac{\exp\left[\frac{(\mu_b N_b + \mu_f N_f - \xi)}{KT}\right]}{\left[2 + \exp\left[\frac{2\varepsilon_j - \mu_b - \mu_f}{KT}\right]\right]} \tag{28}$$

Where Z is the partition function, N_b denotes number of bosons, N_f number of fermions μ_b is the chemical potential of bosons, μ_f is the chemical potential of fermions, T is the temperature, K is the Boltzmann constant. ζ is the dual energy of helium isotopes.

Equation (28) gives the partition function of a grand canonical ensemble of a mixture of helium isotopes with a spin degeneracy of two. It ought to be understood that the partition function has two brackets: the first bracket consists of the difference of the chemical potential of bosons and fermions and a factor 2-times which is due to interaction of bosons and fermions in the mixture. The second bracket comprises of μ_f which means that fermions are not affected by the distribution of the bosons in the mixture because in whichever way the bosons are arranged or distributed, there should only be one fermion.

Internal Energy

For a grand canonical ensemble, internal energy E was derived as

$$E = k\sum_{N_b,N_f}^{\infty}\left[T^2\frac{\partial}{\partial T}\ln\left(2\left[4+2\exp\left(\frac{\mu_b-\mu_f}{KT}\right)+\exp\left[2\left(\frac{-\mu_f+\varepsilon_j}{KT}\right)\right]\right]\frac{\exp\left[\frac{(\mu_b N_b+\mu_f N_f-\xi)}{KT}\right]}{\left[2+\exp\left(\frac{2\varepsilon_j-\mu_b-\mu_f}{KT}\right)\right]}\right)\right] \quad (29)$$

RESULTS AND DISCUSSIONS

Analysis

In this study, we have applied data for a helium binary system as commonly used by Ayodo *et al.*, (2004) to study trends and further undertake a comparative study with the experimentally observed data of the system.

Table 1: Essential parameters for liquid helium-3 and helium-4

	Liquid ^{3}He	**Liquid ^{4}He**
Volume (cm^3)	40.00	28.00
Density (gcm^{-3})	0.07	0.14
Mass (g)	2.80	3.82

Although chemical potential is temperature dependent, at low temperatures, it assumes a nearly constant value given by the expression

$$\mu = \frac{\pi^2\hbar^2}{2m}\left(\frac{3\mathrm{N}}{\pi V}\right)^{2/3} \quad (30)$$

Here, *m* is the molar mass of the species, *V* is its molar volume, and $\mathbf{N}$ is Avogadros number.

The chemical potentials for bosons and fermions are then obtained as

$\mu_f = 3.184 \times 10^{-27}\ eV$ and $\mu_b = 6.215 \times 10^{-28} eV$

In a four-level approximation, higher energy levels lie beyond the ionization potential of helium (≈79.02 eV), Sakwa *et al.*, (2004), where they experience no influence of the nucleus.

Variation of Thermodynamic Quantities with Temperature

Partition Function

Using equation (28) the variation of partition function with temperature was studied in the temperature range 5K to 100K. The transition temperature of pure liquid Helium-4 is about 2.167, Ayodo (2002). The graph depicting the variation of the partition function with the temperature is shown in figure 1 below.

There is a gradual increase in the values of the partition function as the temperature of the system is increased. As the temperature is increased, fermions quickly shift to higher energy levels. Helium-3 shifts the transition temperature of the latter to a higher value Ayodo *et al.*, (2004).

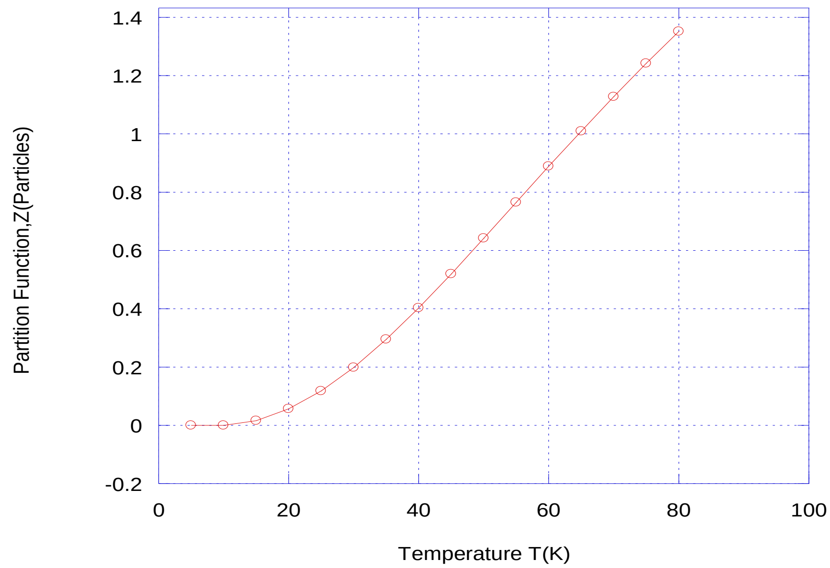

Figure 1: Variation of partition function with temperature in the range of 5K to 100K

Internal Energy

Equation (29) is used to compute the internal energy of the system at varying temperatures from 5K to 100K at intervals of 5K. The variation of internal energy and temperature of the system is depicted in *figure 2* below.

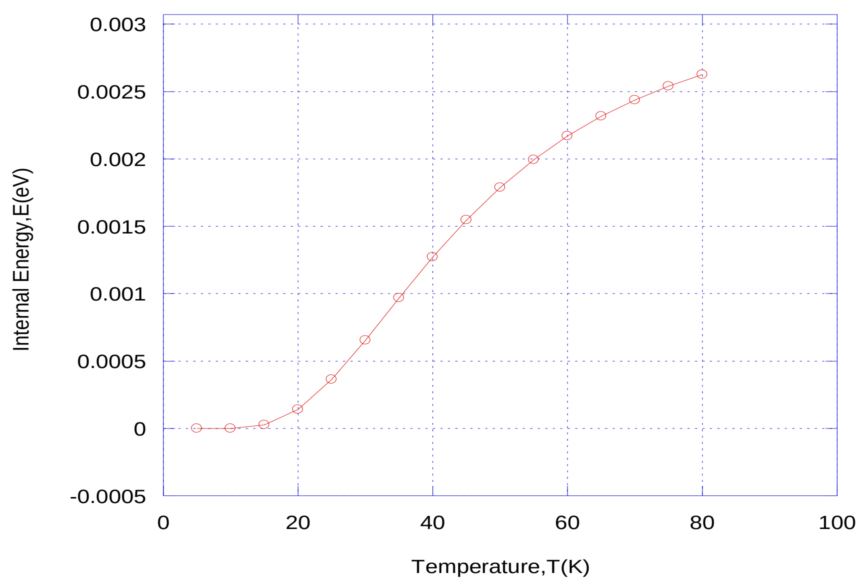

Figure 2: Variation of Internal Energy with Temperature in the temperature range of 5K to 100K

The internal energy approaches zero as temperature tends to zero.In the low temperature regime, particles occupy the lower quantum states. As the temperature is increased, fermions shift quickly to the higher states where they posses greater kinetic energy necessarily manifested as internal energy. The increase in internal energy at higher temperatures declines due to particle saturation.

Conclusions

We have shown that a pair of fermion is a boson because adding the two half integer spins give an integer spin. Therefore at low temperatures, fermions and bosons forms cooper pairs. The movement of this cooper pairs is necessitated by weak interaction of the particles in terms of the oscillation of the lattice. At high temperatures, the particles have a lot of energy and move past each other and this explains why this model of non interacting degenerate works so well. The partition function of this model, like others (Ryan *et al.*,2015), increases exponentially as temperature is increased forming a plateau at higher temperatures. This is because degeneracy inhibits formation of microstates so that even if the temperature is increased, fermions occupancy in any quantum state is limited to two.

At low temperatures (below 5 K), the internal energy of the system approaches zero. In this range of temperatures, most particles are in the ZFC and consequently the internal energy is diminishingly small. These observations agree to a large extent with conventional results about entropy and internal energy for systems with high occupancy of the ZMS (Sakwa et al.,2013), increase in temperature result in an increase in internal energy as is normally the case in thermodynamics.

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