QUANTUM SIZE AND DEGENERACY EFFECTS ON THERMAL SELF-DIFFUSION UNDER FREE MOLECULAR TRANSPORT REGIME

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ABSTRACT

Thermal self-diffusion coefficients of monatomic ideal Fermi and Bose gases (like He3 and He4) are analytically determined by considering quantum size effects (QSE) for free molecular flow regime. The variations of thermal diffusion coefficients for Fermi and Bose gases with chemical potential are analyzed by neglecting QSE to understand the pure effect of quantum degeneracy. The results show that quantum degeneracy causes a substantial difference especially in degeneracy limit. It is seen that quantum degeneracy reduces thermal diffusion rate for both Fermi and Bose gases. There is a limit value for diffusion rate in a completely degenerate Bose gas. Furthermore, diffusion rates for Fermi and Bose gases are different from each other for the same degeneracy level. This difference in diffusion rates can be used for isotopic separation. QSE on thermal diffusion coefficients are also investigated. QSE cause tiny deviations from macroscopic behavior of thermal self-diffusion. QSE have negative contribution on thermal self-diffusion at low degeneracy while an opposite contribution appears at high degeneracy limit. Dimensionless diffusion coefficient goes to unity for a completely degenerate Fermi gas while it goes to infinity for a Bose gas.

INTRODUCTION

Nano Scale transport has a great deal of attention in recent years because of the increasing trend of manufacturing on these scales. Many transport phenomena in macro scale have to be revised or modified since many negligible effects in macro scale can be dominant in nano scale [1-3]. Quantum size effects (QSE) are one of these effects and they arise when thermal de Broglie wavelength of particles is not negligible in comparison with the characteristic size of the system. In such a case, wave character of particles becomes important and make thermodynamic and transport properties depend on shape and size of the domain [4-16].

Quantum degeneracy is another effect, which can be important in case high density or low temperature conditions. Under those conditions, thermal de Broglie wave length of particles is large enough in comparison with the mean distance between particles. Therefore quantum degeneracy becomes important and cause considerable changes in transport behaviours. In this case, quantum statistics (Fermi or Bose) should be used in calculations.

Transport processes in nano domains are generally considered within the scope of free molecular transport regime in which particle wall collisions are dominate instead of particle-particle ones. Therefore, size and surface effects can be more important in free molecular flow regime.

In this paper, thermal self-diffusion in free molecular transport regime is considered and both quantum degeneracy and QSE are taken into account in the calculations. Thermal self-diffusion fluxes of monatomic ideal Fermi and Bose gases (like He3 and He4) are determined. The influences of quantum degeneracy and QSE on thermal self-diffusion rates are examined.

THERMAL-SELF DIFFUSION IN QUANTUM DEGENERACY LIMIT

Thermal self-diffusion coefficient built up a relation between the diffusive flux and the temperature gradient and it is written in the following form

$$\vec{J} = -D_{th}\vec{\nabla}T \qquad (1)$$

Here, D_{th} is the thermal self-diffusion coefficient, J is the particle flux due to temperature gradient, $\vec{\nabla}T$. To examine quantum size effects on thermal self-diffusion, nano scale transport domain is considered. Therefore free molecular transport regime is dominant since the mean free path of particles is usually larger than the characteristic size of the domain at nano scale. For ideal Maxwellian and quantum gases (Fermi and Bose) thermal self-diffusion coefficient can be given for free molecular transport regime as [17];

$$D_{th} = -\frac{\vec{J}}{\vec{\nabla}T} = nL_g\sqrt{\frac{2k_B}{mT}}\frac{g_2}{\eta}\left(1-\Lambda\frac{g_0}{g_2}\right) \qquad (2)$$

In Eq. (2), n is particle density, L_g is the characteristic size of the domain which can be given by $V/2A$ where V and A are domain volume and surface area respectively, k_B is the Boltzmann's constant, T is temperature, m is the particle mass and Λ is the dimensionless chemical potential defined as $\Lambda = \mu/k_BT$ in terms of chemical potential, μ . Definitions of η , g_0 and g_2 functions are given in Refs. [13, 17] and their ratios in Eq.(2) can be obtained for an ideal quantum gases (namely Fermi Dirac-FD and Bose Einstein-BE gases) as follows

$$\frac{g_2}{\eta} = \frac{4}{3\sqrt{\pi}} \frac{Li_2\left[\mp e^{\Lambda}\right]}{Li_{3/2}\left[\mp e^{\Lambda}\right]} \tag{3}$$

$$\frac{g_0}{g_2} = \frac{1}{2} \frac{Li_1\left[\mp e^{\Lambda}\right]}{Li_2\left[\mp e^{\Lambda}\right]} \tag{4}$$

where Li represents the Polylogaritm functions while negative and positive signs stand for Fermi and Bose gases, respectively. The strength of degeneracy increases with increasing value of *Λ*. Completely degenerate Fermi and Bose gases are obtained for the corresponding limits of $\Lambda \to \infty$ and $\Lambda \to {}^{-}0$. In classical limit, $\Lambda \to -\infty$, degeneracy disappears and Polylogarithm functions reduces to $Li\left[\mp e^{\Lambda}\right] \to \mp e^{\Lambda}$. Thus, Eqs. (3) and (4) reduce to the equations given below for an ideal Maxwell gas

$$\frac{g_2}{\eta} = \frac{4}{3\sqrt{\pi}} \tag{5}$$

$$\frac{g_0}{g_2} = \frac{1}{2} \tag{6}$$

To examine the pure quantum degeneracy effects on thermal self-diffusion, dimensionless diffusion coefficient is defined and determined by using Eqs. (3) and (4) in Eq.(2) as

$$\tilde{D}_{th} = \frac{D_{th}}{nL_g\sqrt{\frac{2k_B}{mT}}} = \frac{4}{3\sqrt{\pi}} \frac{Li_2\left[\mp e^{\Lambda}\right]}{Li_{3/2}\left[\mp e^{\Lambda}\right]} \left(1 - \frac{1}{2}\Lambda \frac{Li_1\left[\mp e^{\Lambda}\right]}{Li_2\left[\mp e^{\Lambda}\right]}\right) \tag{7}$$

Degeneracy effects can be analysed for Fermi and Bose gases separately by using the proper value intervals of Λ in Eq.(7). The results are given in Fig. 1.

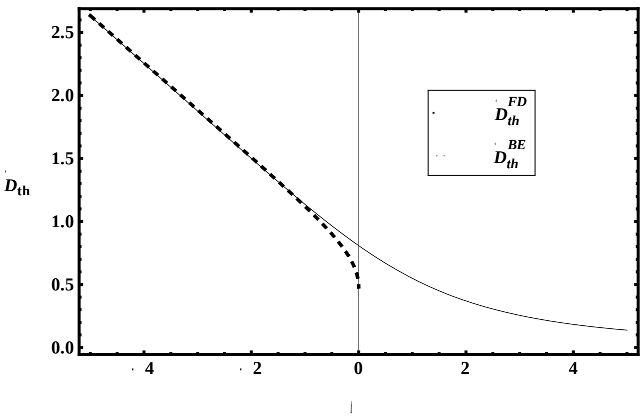

Figure 1: Variation of dimensionless diffusion coefficient with dimensionless chemical potential for Bose (dashed curve) and Fermi (solid curve) gases.

It is seen that quantum degeneracy reduces thermal diffusion rate for both Fermi and Bose gases. Furthermore, diffusion rates for Fermi and Bose gases are different from each other for the same degeneracy level (the same value of Λ). This difference in diffusion rates can be used for isotopic separation if one isotope obeys Fermi statistics while the other one obeys Bose one, like He3 and He4 gases. For a completely degenerate Bose gas ($\Lambda \to {}^{-}0$), by using the asymptotic forms of Polylogarithm functions, it is possible to show that Eq.(7) goes to $4\zeta(2)/3\sqrt{\pi}\,\zeta(3/2) \cong 0.474$. On the other hand, for a completely degenerate Fermi gas, it goes to zero.

SELF-THERMAL DIFFUSION UNDER QUANTUM SIZE EFFECTS

In order to consider quantum size effects, which result from the wave character of particles and may cause considerable changes in transport phenomena at nano scale, it is necessary to calculate the functions of η, g_0 and g_2 more precisely. These calculations have been done in Ref. [17] and the following ratios can be given

$$\frac{g_2}{\eta} = \frac{4}{3\sqrt{\pi}} \frac{Li_2\left[\mp e^{\Lambda}\right]}{Li_{3/2}\left[\mp e^{\Lambda}\right]} \frac{\left[1 - \frac{\alpha}{\sqrt{\pi}} \frac{9\pi}{32} \frac{Li_{3/2}\left[\mp e^{\Lambda}\right]}{Li_2\left[\mp e^{\Lambda}\right]}\right]}{\left[1 - \frac{\alpha}{\sqrt{\pi}} \frac{Li_1\left[\mp e^{\Lambda}\right]}{Li_{3/2}\left[\mp e^{\Lambda}\right]}\right]} \tag{8}$$

$$\frac{g_0}{g_2} = \frac{1}{2} \frac{Li_1\left[\mp e^{\Lambda}\right]}{Li_2\left[\mp e^{\Lambda}\right]} \frac{\left[1 - \frac{\alpha}{\sqrt{\pi}} \frac{3\pi}{8} \frac{Li_{1/2}\left[\mp e^{\Lambda}\right]}{Li_1\left[\mp e^{\Lambda}\right]}\right]}{\left[1 - \frac{\alpha}{\sqrt{\pi}} \frac{9\pi}{32} \frac{Li_{3/2}\left[\mp e^{\Lambda}\right]}{Li_2\left[\mp e^{\Lambda}\right]}\right]} \tag{9}$$

where $\alpha = \alpha_2 + \alpha_3$, α_j is inverse scale factor defined as $\alpha_j = L_c/L_j$, L_c is the half of the most probable de Broglie wave length given by $L_c = h/\left(2\sqrt{2mk_bT}\right)$ and L_j is the domain size in j direction. Since the direction 1 is chosen as a transport direction here, $\alpha_1 = 0$ (there is no confinement in direction 1). It is clear that Eqs.(3) and (4) can easily be recovered from Eqs. (8) and (9) when domain sizes in directions 2 and 3 are larger enough in comparison with L_c, $\{\alpha_2, \alpha_3\} \to 0$.

To examine the pure quantum size effects on thermal self-diffusion rate, a dimensionless diffusion coefficient for quantum gases is defined as the ratio of diffusion coefficient with and without QSE. By using Eqs.(8) and (9) as well as Eqs.(3) and (4) in Eq.(2), dimensionless diffusion coefficient is obtained as

$$\tilde{D}_{th}^{QSE} = \frac{D_{th,QSE}^{FD/BE}}{D_{th}^{FD/BE}} = \left[\frac{1 - \frac{\alpha}{\sqrt{\pi}} \frac{9\pi}{32} \frac{Li_{3/2}\left[\mp e^{\Lambda}\right]}{Li_2\left[\mp e^{\Lambda}\right]}}{1 - \frac{\alpha}{\sqrt{\pi}} \frac{Li_1\left[\mp e^{\Lambda}\right]}{Li_{3/2}\left[\mp e^{\Lambda}\right]}}\right] \frac{\left[1 - \frac{1}{2}\Lambda \frac{Li_1\left[\mp e^{\Lambda}\right]}{Li_2\left[\mp e^{\Lambda}\right]} \frac{1 - \frac{\alpha}{\sqrt{\pi}} \frac{3\pi}{8} \frac{Li_{1/2}\left[\mp e^{\Lambda}\right]}{Li_1\left[\mp e^{\Lambda}\right]}}{1 - \frac{\alpha}{\sqrt{\pi}} \frac{9\pi}{32} \frac{Li_{3/2}\left[\mp e^{\Lambda}\right]}{Li_2\left[\mp e^{\Lambda}\right]}}\right]}{1 - \frac{1}{2}\Lambda \frac{Li_1\left[\mp e^{\Lambda}\right]}{Li_2\left[\mp e^{\Lambda}\right]}} \tag{10}$$

Equation (10) can be used to analyse QSE on thermal self-diffusion rate for Fermi and Bose gases as well as Maxwell gas by using the proper Λ values. The variation of dimensionless diffusion coefficient with dimensionless chemical potential is seen in Fig.2 for $\alpha = \alpha_2 + \alpha_3 = 0.1$.

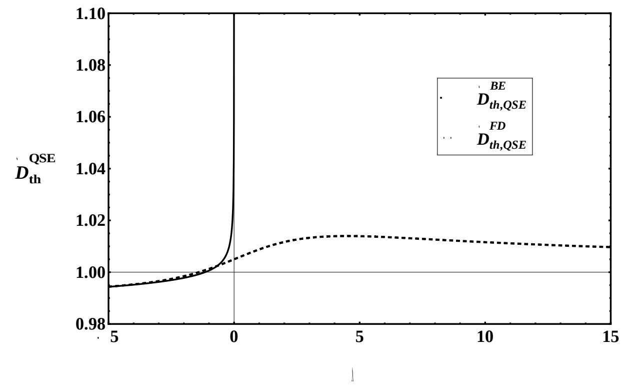

Figure 2: The variation of dimensionless diffusion coefficient with dimensionless chemical potential for $\alpha = 0.1$.

Fig. 2 shows that QSE cause tiny deviations from macroscopic behavior of thermal self-diffusion. QSE have negative contribution on thermal self-diffusion at low degeneracy or classical limit ($\Lambda \to -\infty$), while an opposite contribution appears at high degeneracy limit. Dimensionless diffusion coefficient goes to unity for a completely degenerate Fermi gas while it goes to infinity for Bose gas. In Maxwellian limit ($\Lambda \to -\infty$), Eq.(10) can be simplified by using the asymptotic forms of Polylogarithm functions, $Li\left[\mp e^{\Lambda}\right] \to \mp e^{\Lambda}$, as

$$\tilde{D}_{th,QSE}^{MB} = \frac{D_{th,QSE}^{MB}}{D_{th}^{MB}} = \left[\frac{1-\frac{\alpha}{\sqrt{\pi}}\frac{9\pi}{32}}{1-\frac{\alpha}{\sqrt{\pi}}}\right]\left[\frac{1-\frac{1}{2}\Lambda\frac{1-\frac{\alpha}{\sqrt{\pi}}\frac{3\pi}{8}}{1-\frac{\alpha}{\sqrt{\pi}}\frac{9\pi}{32}}}{1-\frac{1}{2}\Lambda}\right] \tag{11}$$

CONCLUSION

The results show that quantum degeneracy decreases thermal self-diffusion rate. There is a limit value for diffusion rate in a completely degenerate Bose gas. On the other hand, diffusion rate goes to zero in degeneracy limit for a Fermi gas. Different diffusion rates of Fermi and Bose gases for the same degeneracy level may allow to design an isotopic enrichment process if one isotope obeys Fermi statistics while the other one obeys Bose one, like He3 and He4 gases.

Although quantum degeneracy causes a considerable difference in diffusion rate, only tiny deviations from macroscopic behavior of thermal self-diffusion arises due to QSE. On the other hand, opposite contributions of QSE on diffusion rates of Fermi and Bose gases are also obtained for strongly degenerate limit. Therefore, QSE may also be used for isotopic enrichments.

A possible experimental verification of QSE on thermal self-diffusion rate can be a macroscopic manifestation of wave nature of particles in diffusion process. The results may be used to design some new devices and processes.

NOMENCLATURE

Symbol	Quantity	SI Unit
D_{th}	Thermal self-diffusion coefficient	$m^{-1}.s^{-1}.K^{-1}$
J	Particle flux	(# of particle)$\cdot m^{-2}\cdot s^{-1}$
k_B	Boltzmann's constant	J K^{-1}
L_c	Half of the most probable wave length	m
L_g	Characteristic size of the domain	m
L_j	Size of the domain in direction j	m
n	Particle density	# / m^3
m	Particle mass	kg
T	Temperature	K
α	Dimensionless inverse scale factor	
Λ	Dimensionless chemical potential	
μ	Chemical potential	Joule
BE	Bose-Einstein statistics	
FD	Fermi-Dirac statistics	
MB	Maxwell-Boltzmann statistics	
QSE	Quantum size effect	

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