SCATTERING PROPERTIES OF SPIN-POLARIZED ATOMIC TRITIUM

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Abstract:

In this paper, the Lippmann-Schwinger (LS) formalism is applied to spin-polarized atomic tritium (T↓). The total and viscosity cross sections of T↓- T↓ collisions are calculated, using two triplet-state potentials: a Morse- and a Silvera- type potentials. Also, the scattering length and the binding energy of T↓ atoms are calculated. Our results are found to be in good agreement with previous calculations. Our results for the Morse potential are smaller in magnitude than those for the Silvera potential, because the Morse-potential well is shallower than that of the Silvera potential. In the low-energy limit, the cross sections are dominated by S-wave scattering. In this limit, the S-wave scattering length $a_0 < 0$ for both potentials. This means that the interaction between the T↓ atoms is attractive. The Ramsauer-Townsend (RT) effect and phase transitions in the cross sections are found at low temperatures. The effect of the D-wave scattering appears as a resonance-like behavior in the total cross section. This peak corresponds to a quasi-bound state.

Keywords: Spin-polarized tritium, Total and viscosity cross sections**,** Ramsauer-Townsend effect, Scattering length.

1. Introduction

Spin-polarized tritium (T↓) is an interesting quantum many-body system which obeys Bose statistics. It is expected to be liquid at zero temperature and pressure (Etters et al., 1975; Miller and Nosanow, 1976; Joudeh et al., 2007), thanks to its larger mass. Stwaley and Nosanow (1976) suggested that T↓ should behave very much like ^{4}He, and therefore constitute another example of a bosonic superfluid (Stwaley and Nosanow, 1976).

Various microscopic methods have been adopted for studying this system. First there has been the variational track, including Monte Carlo simulation (Blume et al., 2002; Bešlić et al., 2008; Bešlić et al., 2009; Stipanović et al., 2011) and the lowest-order constrained variational method (Hangen and Østgaard, 1989). Blume et al. (2002) used the Diffusion Monte Carlo (DMC) method to study the microscopic properties of tritium clusters with up to N=40 atoms and compared them to bosonic ^{4}He clusters. In that work, it is shown that (T↓) clusters are more weakly-bound and diluted than ^{4}He clusters with the same number of atoms. In addition, they have shown that the trimer $(T\downarrow)_3$ is the smallest spin-polarized tritium cluster with a ground state-energy of only -4.2(7) mK. The stability of mixed clusters of T↓ with spin-polarized hydrogen (H↓) and spin-polarized deuterium (D↓) has also been investigated (Bešlić et al., 2009; Stipanović et al., 2011). For the clusters with D↓, the stability limits depend on the number of D↓ atoms and the occupation of its nuclear spin states. On the other hand, because of the small mass of H↓, it has been shown that even 60 T↓ atoms are not enough to bind one H↓ atom. Second, there has been the perturbative track (Solís et al., 1993). The ground-state properties of the spin-polarized bosonic fluids H↓ and T↓ have been determined using a quantum thermodynamic perturbation theory, with emphasis on the repulsive-sphere gas.

In this work, we shall apply the Lippmann-Schwinger (LS) formalism to our system so as to calculate the cross sections, and then the Ramsauer-Townsend (RT) effect and phase transitions in T↓-T↓ scattering will be explored. RT effect is the phenomenon occurring in the collision between two particles when the total cross section is a minimum at a particular value of the relative energy (Borghesani, 2001). Also, the S-wave scattering length and then the binding energy of T↓ will be calculated at very low energy.

We consider an extended system consisting of N spin-polarized tritium atoms, each of mass m, occupying a volume Ω at zero temperature and pressure such that the particle density is given by $\rho = N/\Omega$ and in a very-large magnetic field of order 10 T. The system is assumed to interact through the triplet-state potential.

The rest of the paper is organized as follows. The underlying theoretical framework is presented in Section 2. The results are summarized and discussed in Section 3. Finally, Section 4 comprises a summary of our results and the main conclusions.

2. Cross Sections of T↓-T↓ Scattering

The basic elements of the theory of scattering by a potential V(r), where r is the interatomic distance, are one known. We have already distilled the necessary equations and expressions for our present purposes in a previous publication (Al-Maaitah et al., 2011).

However, for reference purposes as well as to establish our notation, we summarize here the necessary expressions.

In compact form, a general expression for the integral cross sections may be defined by (Merzbacher, 1998)

$$\sigma_n = 2\pi\int_0^{\pi}\left(1-\cos^n\theta\right)\frac{d\sigma}{d\Omega}(\theta)\sin\theta\, d\theta, \tag{1}$$

where n = 1 corresponds to the diffusion cross section σ_D, and n=2 to the viscosity cross section σ_η; θ is the center-of-mass scattering angle, and $\frac{d\sigma}{d\Omega}(\theta)$ is the differential cross section.

If the force causing the scattering is central, $\frac{d\sigma}{d\Omega}(\theta)$ for bosons is given by

$$\frac{d\sigma}{d\Omega}(\theta) = \left|f(\theta)+f(\pi-\theta)\right|^2 \tag{2}$$

$f(\theta)$ being the scattering amplitude and is defined by (Landau,1996)

$$f(\theta) = \frac{1}{2ik}\sum_{\ell=0}^{\infty}(2\ell+1)\left[\exp\left(2i\delta_\ell(k;P,\beta)\right)-1\right]P_\ell(\cos\theta), \tag{3}$$

$P_\ell(\cos\theta)$ being the first-kind Lengendre polynomial of order ℓ.

The total cross section σ_T is given by

$$\sigma_T = 2\pi\int_0^{\pi}\frac{d\sigma}{d\Omega}\sin\theta\, d\theta \tag{4}$$

Substituting n = 1 in Eq. (1), we have

$$\sigma_D = 2\pi\int_0^{\pi}\left(1-\cos\theta\right)\frac{d\sigma}{d\Omega}(\theta)\sin\theta\, d\theta. \tag{5}$$

The first integral is even; whereas the second is odd and therefore vanishes. It follows that

$$\sigma_D = 2\pi\int_0^{\pi}\frac{d\sigma}{d\Omega}(\theta)\sin\theta\, d\theta = \sigma_T \tag{6}$$

Substituting Eq. (3) in Eq.(6), we have

$$\sigma_T = \sigma_D = \frac{4\pi}{k^2}\sum_{\ell=0}^{\infty}(2\ell+1)\left(1+(-1)^{\ell}\right)\sin^2\delta_{\ell} \quad . \qquad . \qquad (7)$$

The viscosity cross section σ_{η} is obtained by substituting n = 2 in Eq. (1):

$$\sigma_{\eta} = \frac{4\pi}{k^2}\sum_{\ell=0}^{\infty}\frac{(\ell+1)(\ell+2)}{\left(\ell+\frac{3}{2}\right)}\left(1+(-1)^{\ell}\right)\sin^2\left(\delta_{\ell+2}(k)-\delta_{\ell}(k)\right). \qquad (8)$$

The total cross section for spin-polarized bose atoms (Jamieson et al., 1999) is given by

$$\sigma_T = \sigma_D = \frac{8\pi}{k^2}\sum_{\ell(\text{even})}^{\infty}(2\ell+1)\sin^2\delta_{\ell}\,, \qquad (9)$$

Then, the viscosity cross section σ_{η} for spin-polarized bose atoms is given by

$$\sigma_{\eta} = \frac{8\pi}{k^2}\sum_{\ell(\text{even})}^{\infty}\frac{(\ell+1)(\ell+2)}{\left(\ell+\frac{3}{2}\right)}\sin^2\left(\delta_{\ell+2}(k)-\delta_{\ell}(k)\right). \qquad (10)$$

The starting point in computing the T↓-T↓ cross sections is the determination of the relative phase shifts. This can be done by solving the Lippmann-Schwinger (LS) integral equation using a matrix-inversion technique (Bishop et al.,1977).

The Lippmann-Schwinger (LS) t-matrix which best describes two-body scattering in vacuum may be written as (Bishop et al., 1977, Joudeh et al., 2010, Joudeh , 2011):

$$t_{\ell}\left(\vec{p},\vec{p}\,';s,\vec{P}\right) = u\left(\left|\vec{p}-\vec{p}\,'\right|\right) + (2\pi)^{-3}\int d\vec{k}\,u_{\ell}\left(\left|\vec{p}-\vec{k}\right|\right)g_0\left(\vec{k},s\right)t_{\ell}\left(\vec{k},\vec{p}\,';s,\vec{P}\right). \qquad (11)$$

Here: the operator $u \equiv \frac{2\mu}{\hbar^2}V \equiv \frac{1}{2}V$, where V is the Fourier transform of a static central tow-body potential and μ is the reduced mass of the interacting pair: $\mu = \frac{1}{2}m$. Throughout this work we shall use units such that $\hbar = 2m = k_B = 1$, k_B being Boltzmann's constant. The conversion factor being $\frac{\hbar^2}{m} = 16.085\ \text{K Å}^2$. The other parameters shown explicitly in the t-matrix equation-namely, $\vec{p}$, $\vec{p}\,'$, $\vec{P}$ and s denote, respectively, the relative incoming momentum, the relative outgoing momentum, the center of mass

momentum, the total energy of the interacting pair in the center-of-mass frame and is given by

$$s \equiv 2\mu\left(2P_0 - \frac{P^2}{m}\right); \tag{12}$$

P_0 is the kinetic energy of the pair; P^2 is the energy carried by the center of mass.

Using our system of units, we have

$$s = P_0 - P^2. \tag{13}$$

The free two-body Green's function $g_0(s)$ is defined as (Joudeh et al., 2010):

$$g_0(\vec{k}, s) \equiv \frac{1}{k^2 - s - i\eta}\ . \tag{14}$$

The system of interacting real particles is described in terms of weakly interacting quasiparticles; this justifies the use of free Green's functions. The quantity η is a positive infinitesimal in the scattering region and zero otherwise.

To calculate the real and imaginary parts of the t-matrix, it is convenient to define a real K-matrix:

$$K_\ell(\vec{p}, \vec{p}'; s, \vec{P}) \equiv u_\ell(\vec{p}, \vec{p}') - \frac{1}{2\pi^2}\int_0^\infty d\vec{k}\,\frac{k^2 u_\ell(\vec{p}, \vec{k}; s) K_\ell(\vec{k}, \vec{p}'; s) - s\, u_\ell(\vec{p}, \vec{k}) K_\ell(\kappa, \vec{p}'; s)}{k^2 - s}; \tag{15}$$

The relative phase shift $\delta_\ell(p)$ can now be obtained from the parameterization

$$K_\ell(\vec{p}, \vec{p}; p^2) = \frac{-4\pi}{p}\tan\delta_\ell(p). \tag{16}$$

The $s-$wave scattering length a_0 for spin-polarized systems at low energy is defined as (Landau, 1987; Sakurai, 1987)

$$a_0 \equiv -\lim_{k\to 0}\frac{\tan\delta_0(k)}{k} \tag{17}$$

The basic input in our present framework is the triplet-state potential. It is convenient to separate the pair potential V (r) into repulsive and attractive parts (Solís et al., 1993):

$$V(r) = V_{rep}(r) + \lambda V_{att}(r) \qquad 0 \le \lambda \le 1 \qquad (18)$$

where $V_{att}(r)$ is negative and λ=1 corresponds to the full interaction. Here we have used two forms for the triplet-state potential. The first is Morse (Dugan et al.,1973) :

$$V_M(r) = \varepsilon\left[\exp 2c\left(1-\frac{r}{r_m}\right) - 2\exp c\left(1-\frac{r}{r_m}\right)\right], \qquad (19)$$

where $\varepsilon = 6.19$ K; $r_m = 4.1527$ Å is the position of the potential minimum; and $c = 6.0458$ is a dimensionless constant.

The second is Silvera (Silvera, 1980):

$$V_S(r) = \varepsilon V^*(x)$$

$$V^*(x) = A\exp(c_0 - c_1 x - c_2 x^2) - \left(\frac{c_6}{x^6} + \frac{c_8}{x^8} + \frac{c_{10}}{x^{10}}\right)F(x), \qquad (20)$$

$$F(x) = \begin{cases} \exp\left[-\left(\frac{D}{x}-1\right)^2\right], & x < D, \\ 1, & x \ge D, \end{cases} \qquad (21)$$

$x \equiv r/r_m$; $r_m = 4.16$ Å; $\varepsilon = 6.46$ K; $A = 4.889\times10^4$; $c_0 = 0.0968$; $c_1 = 8.6403$; $c_2 = 2.427$; $c_6 = 1.365$; $c_8 = 0.425$; $c_{10} = 0.183$ and $D = 1.28$.

3. Results and Discussion

Our results are calculated using the Morse and Silvera triplet-state potential. The (LS) t-matrix, which can be considered as the pairwise interaction in momentum space, was determined using a matrix-inversion technique (Ghassib et al.,1976). In all Gaussian-quadrature integrations, a 96-mesh points was used to give accurate results. The total (=diffusion) and viscosity cross sections for T↓- T↓ scattering are calculated using Eqs. (9) and (10), respectively. It was found to be necessary to include partial waves up to $\ell = 14$ to obtain results accurate to better than ~ 0.5%.

Figure 1 displays the total cross section σ_T for T↓- T↓ scattering as a function of k in vacuum [LS], using both the Morse and Silvera potentials. At small energies the total cross section satisfies the condition of the Ramsauer-Townsend (RT) effect. σ_T shows a deep minimum at k~ 0.26 $Å^{-1}$ and 0.28 $Å^{-1}$ for Morse and Silvera potentials, respectively. This minimum appears as a result of a delicate balance between attractive short-range and repulsive zero-range interactions. The physical observation is that, at a particular value of the T↓- T↓ collision energy, the total scattering cross section is anomalously small; or equivalently, the mean free path of T↓ atoms is correspondingly large. At this energy, therefore, T↓ atoms propagate as essentially free, unscattered particles. Our results for RT effect are summarized in Table 1. The peak in σ_T (resonance-like behavior) for Morse potential is smaller in magnitude than that for the Silvera potential, as shown in Table 2. This peak may be interpreted as an indicator of a quasi-bound state (Alm et al., 1994, Sandouqa et al., 2010).

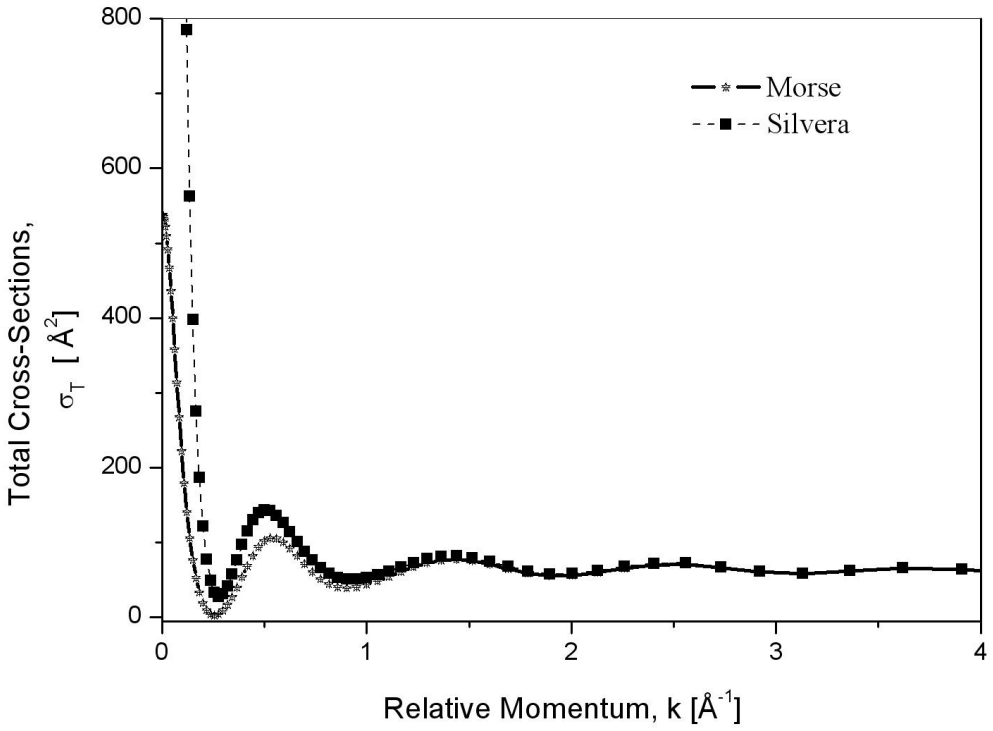

Figure 1: The total cross section σ_T [$Å^2$] for T↓- T↓ scattering as a function of k [$Å^{-1}$] in vacuum [LS], using the Morse potential and the Silvera potential.

Table 1: The Ramsauer-Townsend total cross section σ_T [Å^2] for T↓- T↓ scattering using the Morse and Silvera potentials in vacuum [LS].

Triplet-state potential	σ_T [Å^2]
Morse	2.50
Silvera	27.93

Table 2: The peak in the total cross section σ_T [Å^2] for T↓- T↓ scattering using the Morse and Silvera potentials in vacuum [LS].

Triplet-state potential	σ_T [Å^2]
Morse	105.12
Silvera	143.94

Figure 2 displays the viscosity cross section σ_η for T↓- T↓ scattering as a function of k in vacuum , using both the Morse and Silvera potentials. σ_η has the same behavior as the total cross section, i.e., they have an RT minimum and a resonance-like behavior. Table 3 shows σ_T (0) and σ_η(0) for the Morse and the Silvera potentials. Our results for the Morse potential are smaller in magnitude than those for the Silvera potential, because the Morse-potential well is shallower than that of the Silvera potential.

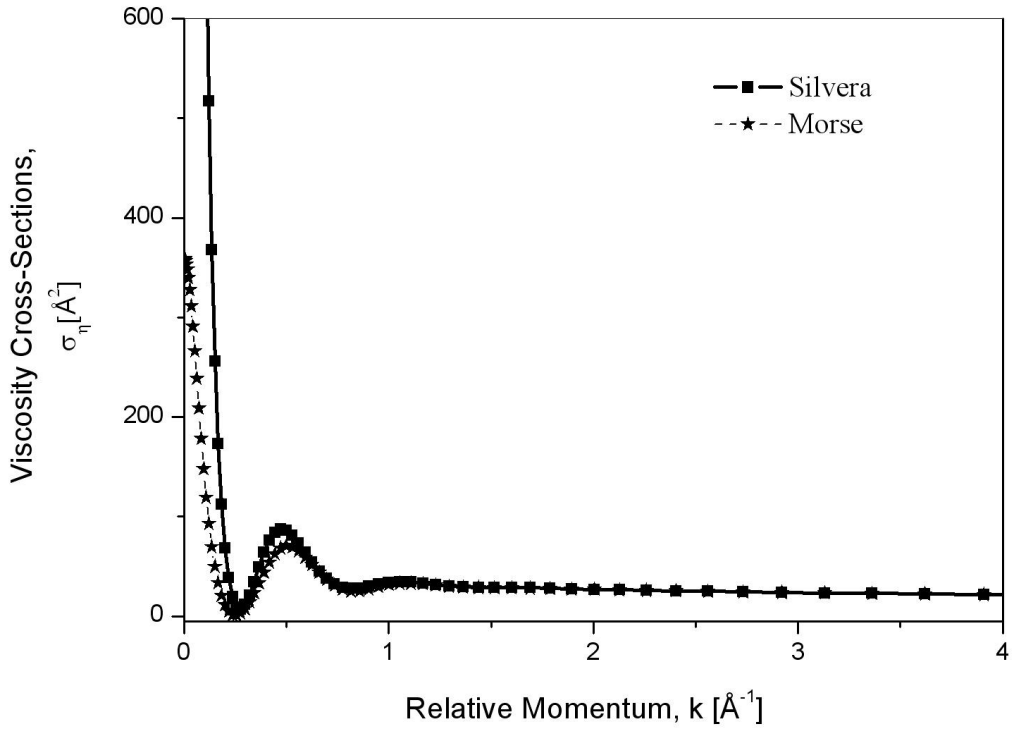

Figure 2: The viscosity cross section σ_η [Å^2] for T↓- T↓ scattering as a function of k [Å^{-1}] in vacuum [LS], using the Morse potential and the Silvera potential.

Table 3: σ_T (0) [Å^2] and σ_η(0) [Å^2] for T↓- T↓ scattering using the Morse and Silvera potentials in vacuum [LS].

Triplet-state potential	σ_T(0) [Å^2]	σ_η(0) [Å^2]
Morse	538.42	358.95
Silvera	33213.20	22142.14

Figures 3 and 4 represent the S-wave cross section σ_0 and the total cross section σ_T as a function of k in vacuum using the Morse and the Silvera potentials, respectively. From these two figures, it is noted that the S-wave is the most significant partial scattering contributing to the total cross section at low energy. Therefore, the RT minimum arises

because S-scattering becomes small. The S-wave scattering length a_0, which is the most important parameter governing the interactions of low-energy atoms, has been calculated for our system at low energy using the Morse and Silvera triplet-state potentials, as shown in Table 4. It is noted that the S-wave scattering length $a_0 < 0$ for both potentials, this means that the interaction between T↓ atoms is attractive. These results are in good agreement with those obtained by (Blume et al., 2002). The negative scattering length suggests the existence of a bound state for T↓ atoms. The binding energy E_B for two types of T↓- T↓ interaction potentials can be determined using $(E_B = \hbar^2/m a_0^2)$. Our results for E_B are presented in Table 4. It is noted that the value of E_B depends on the type of the interaction potential employed. Our results for E_B using the Morse and the Silvera potentials are in good agreement with the previous calculations (Etters et al.,1975, Joudeh et al., 2007) and (Blume et al., 2002), respectively.

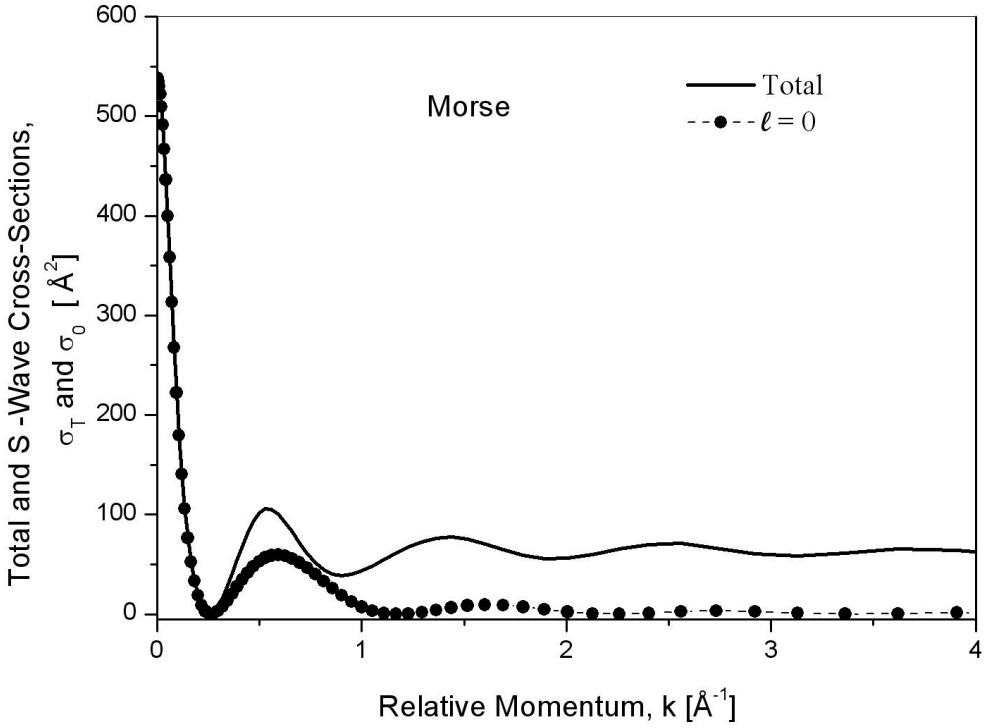

Figure 3: The S-wave cross section $\sigma_0[Å^2]$ and the total cross section σ_T for T↓- T↓ scattering as a function of k [$Å^{-1}$] in vacuum [LS], using the Morse potential.

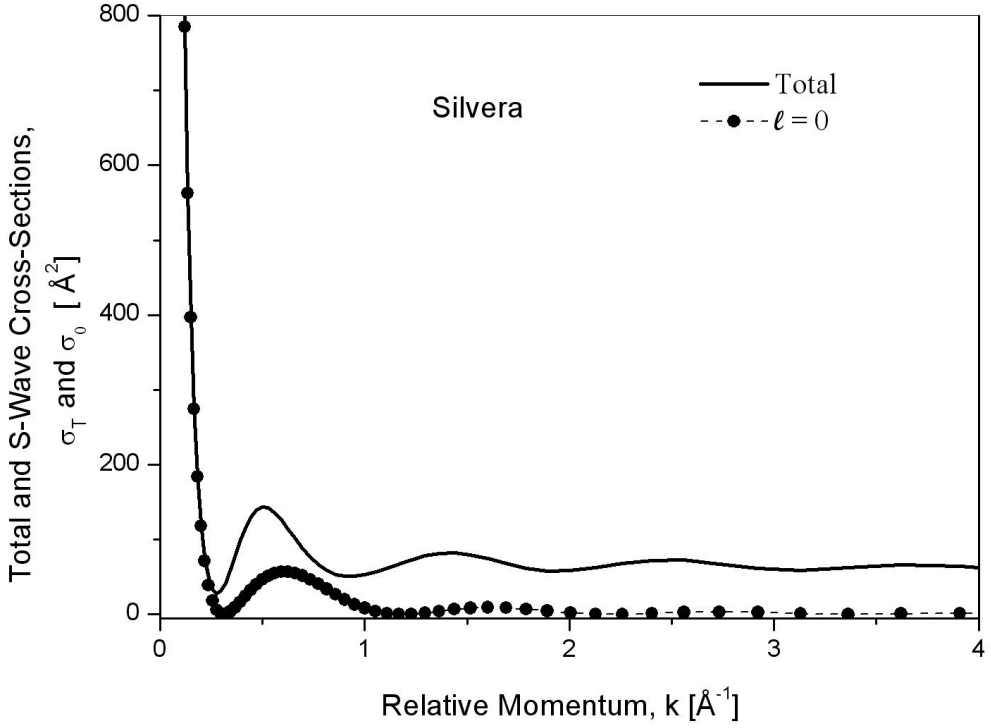

Figure 4: The S-wave cross section σ_0[Å^2] and the total cross section σ_T for T↓- T↓ scattering as a function of k [Å^{-1}] in vacuum [LS], using the Silvera potential.

Table 4: The S-wave scattering length a_o[Å] and the binding energy E_B(K) of the weakly bound tritium using the Morse and Silvera potentials.

Triplet-state potential	a_o[Å]	E_B(K)
Morse	-4.628	0.75 [0.75(2)][a] [0.75][b]
Silvera	-36.367 [-42.692][c]	0.012 [0.0042(7)][c]

[a][Etters et al.,1975]

[b][Joudeh et al., 2007]

[c][Blume et al., 2002]

Figures 5 and 6 show the behavior of the total cross section σ_T and the ℓ – wave cross section (ℓ=0, 2) for T↓-T↓ scattering as a function of k in vacuum, using the Morse and

Silvera potentials. The odd partial waves are absent in the Bose-Einstein statistics (Aldridge and Davis, 1967, Joudeh et al., 2010). In the low-energy limit ($k < 0.3$ Å^{-1}) the D-wave($\ell=2$) cross section is negligible compared to that of the S-wave and with increasing k (increasing energy) σ_0 tends to decrease; but this decrease is overcome by the higher partial-wave contributions, especially the D-wave, which initially increase with energy from zero before passing through a maximum, and then begin to decrease. Sharper structures are due to shape resonances. The most prominent is the D-wave resonance corresponds to a quasi-bound state trapped by the $\ell=2$ centrifugal barrier. This resonance occurs at k~ 0.56 Å^{-1} and 0.50 Å^{-1} for Morse and Silvera potentials, respectively. For k>1Å^{-1}, σ_T is nearly constant. The oscillatory behavior of the cross section as a function of momentum is clearly observed into the high-energy region and originates from the indistinguishability of the T↓ atoms, which are scattered by the repulsive part of the potential (Cantini et al., 1972; Feltgen et al., 1982). The amplitude of the oscillations decreases in the first approximation as the inverse of the relative velocity of the colliding atoms (Dondi et al., 1969; Cantini et al., 1972). This behavior was first noticed by Bernstein (1963) who also pointed out that the number of oscillations was related (semiclassically) to the number of bound states of the potential.

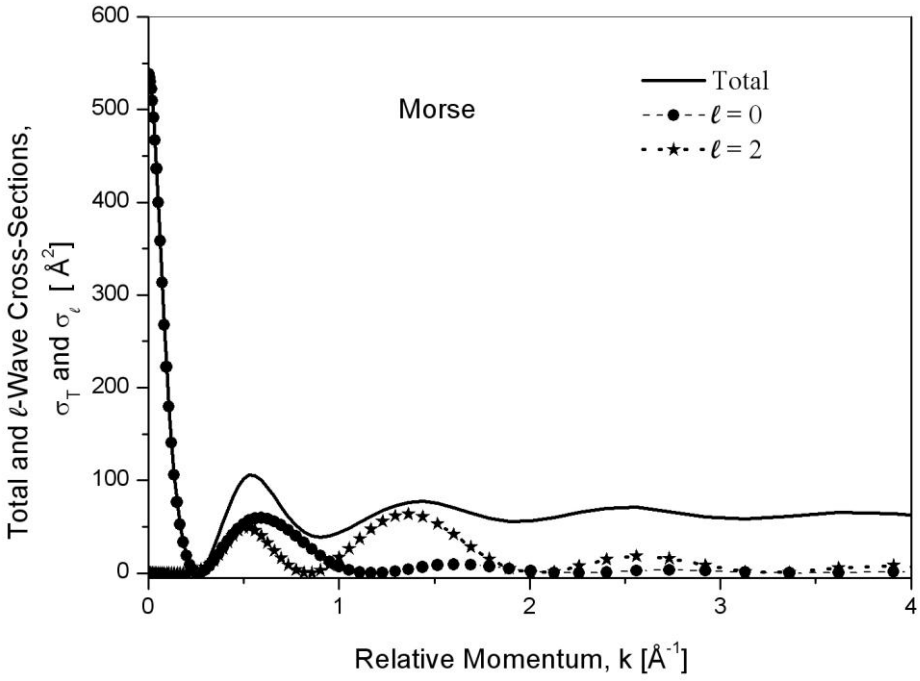

Figure 5: The total cross section σ_T and the $\ell-$wave cross section ($\ell=0,2$) for T↓- T↓ scattering as a function of k [Å^{-1}] in vacuum[LS], using the Morse potential.

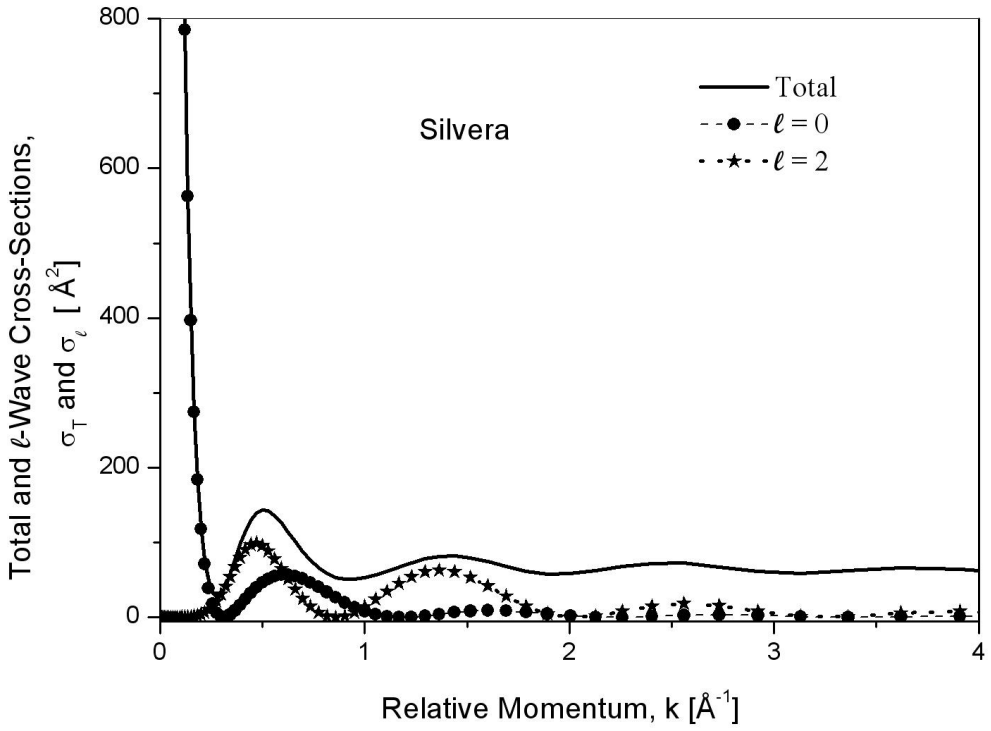

Figure 6: The total cross section σ_T and the $\ell-$wave cross section (ℓ=0,2) for T↓- T↓ scattering as a function of k [$Å^{-1}$] in vacuum[LS], using the Silvera potential.

4. Conclusion

In this paper, the cross sections of T↓- T↓ collisions are calculated, namely, the total and viscosity cross sections, using two triplet-state potentials: a Morse- and a Silvera- type potentials. The achievements of the paper are: (1) the prediction of the Ramsauer-Townsend effect in this system; (2) the prediction of a phase transition due to resonance-like behavior in the total cross section; (3) the calculation of the S-wave scattering length and (4) the calculation of binding energy of spin-polarized tritium using both potentials.

In the low-energy limit, the cross sections are dominated by S-wave scattering. In this limit, the S-wave scattering length $a_0 < 0$ for both potentials, this means that the interaction between the T↓ atoms is attractive. The effect of the D-wave scattering appears as a resonance-like behavior on the total cross section. Our results for the Morse potential are smaller in magnitude than those for the Silvera potential, because the Morse-potential well is shallower than that of the Silvera potential.

In conclusion, our calculations for cross sections show that these quantities are useful indicators of quasi-bound states in spin polarized tritium atoms and how sensitive the scattering length of T↓- T↓ collisions is to the potential employed.

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