Advances in Applied Physics, Vol. 6, 2018, no. 1, 1 - 8
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https://doi.org/10.12988/aap.2018.71210

Scattering Properties for Krypton-86 Gas

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Abstract

In our paper, a theoretical model is introduced to calculate the effective phase shifts, and then the effective total cross section, the effective scattering length and the binding energy for krypton gas at different temperatures and different densities. This model is based on the Galitskii-Migdal-Feynman (GMF) formalism which is essentially an independent-pair model in the presence of a many-body medium. The interaction potential in our work is the Hartree-Fock dispersion (HFD-B) potential.

Keywords: Galitskii-Migdal-Feynman; scattering; crosssection; scattering length

Introduction

Scattering theory is a framework for studying and understanding the interaction or scattering of solutions to partial differential equations. Both classical and quantum mechanical scattering phenomena are characterized by the scattering cross section, σ. The concept of cross section, is that of effective area for collision. The scattering potential representing the Kr-Kr interaction is taken in the present work as the HFD-B potential [1]. The properties of the interatomic krypton potential are:(i) The repulsive term, describes Pauli repulsion at short ranges due to overlapping electron orbitals; (ii) The attractive long-range term, describes attraction at long ranges; (iii) The interaction energy is a minimum at the equilibrium position. Using a scattering T-matrix; which is the basic quantity in the GMF formalism to calculate the 'effective' phase shifts that incorporate many-body effects [4]. Krypton is a member of group 18 (noble gases) elements. A colorless, odorless, tasteless noble gas, krypton occurs in trace amounts in the atmosphere and is often used with other rare gases in fluorescent lamps. Several theoretical and experimental methods have been developed to study the Krypton gas: Total cross sections for excitation by electron impact of metastable states in the noble gases helium, neon, argon, krypton, and xenon have been measured as a

function of impact energies[7]. Approximate differential cross sections for elastic collisions of rare gas ions with their parent atoms are proposed for He+-He, Ne+-Ne, Ar+-Ar, Kr+-Kr, and Xe+-Xe collisions for collision energies from ~ 0.1 eV to 10 keV [5]. In our work, the first step in the GMF formalism was to determine the many-body phase shifts, this by solving GMF integral equation using a matrix-inversion technique.

Interaction Potential

Krypton has a fully occupied *d*-shell in its electronic structure, which makes an accurate calculation of the interaction potential computationally expensive. The two-body potential representing the Kr-Kr interaction is taken in the present work as the HFD-B potential [1], given by $V(r)=\varepsilon V^*(x)$, where

$$V^*(x)=A^*\exp\left(-\alpha^* x+\beta^* x^2\right)-F(x)\sum_{j=0}^{2} c_{2j+6}/x^{2j+6} \tag{1}$$

$$F(x)=\begin{cases}\exp-\left[\left\{\dfrac{D}{x}-1\right\}^2\right], & x<D\\ 1, & x>D\end{cases} \qquad x\equiv\frac{r}{r_m};$$

r_m=4.008 Å A*=1.10146811; α*=9.39490495; β*=-2.32607647; D=1.28; C_6=1.08822526; C_8 = 0.53911567; C_{10} = 0.42174119; ε/k_B = 201.2K.

We begin with the T- matrix which is given by a Bethe-Salpeter-like equation [9,3]:

$$\begin{aligned}&T(\vec{p},\vec{p}';s,\vec{P},\beta)=u(|\vec{p}-\vec{p}'|)-(2\pi)^{-3}\int d\vec{k}\,u(|\vec{p}-\vec{k}|)\\ &\times\left[g_0(k,s)Q(\vec{k},\vec{P},\beta)-g_0^{+}(k,s)\overline{Q}(\vec{k},\vec{P},\beta)\right]T(\vec{k},\vec{p}';s,\vec{P},\beta)\end{aligned} \tag{2}$$

Here: p and p' are the relative incoming and outgoing momenta; P is the center-of-mass momentum. The operator $u\equiv\frac{2m_rV}{\hbar^2}\equiv\frac{1}{2}V$ [in natural units] m_r being the reduced mass of the Kr interacting pair: $m_r=\frac{1}{2}m$, and V the Fourier transform of a static central two-body potential. The free two-body Green's function go(s) is specified by $g_0(\vec{k},s)\equiv\frac{1}{k^2-s-i\eta}$, η being a positive infinitesimal in the scattering region (s>0) and zero otherwise, and the parameter s the total energy of the interacting pair in the center-of-mass frame, given by $s\equiv 2\mu\left(2P_o-\frac{P^2}{m}\right)$, (3)

P_0 is the total energy of the pair and P^2 is the energy carried by the center of mass. For a many-bosonic system, the operator $Q(\overline{Q})$ is the product of two occupation probabilities as follows [10]:

$$Q(k,P,\beta)=\left(1+n\left(\left|\vec{k}-\vec{P}\right|\right)\right)\left(1+n\left(\left|\vec{k}+\vec{P}\right|\right)\right); \tag{4}$$

$$\overline{Q}(k,P,\beta)=n\left(\left|\vec{k}-\vec{P}\right|\right)n\left(\left|\vec{k}+\vec{P}\right|\right). \tag{5}$$

where $n(\vec{k})$ is the Bose-Einstein distribution, given by: $n(\varepsilon)=\dfrac{1}{e^{\beta(\varepsilon-\mu)}-1}$ (6)

The chemical potential μ is given by $\mu=k_BT\ln\left(\dfrac{n}{n_q}\right)$ (7)

Upon partial-wave decomposition, Eq. (2) takes the form [11]

$$T_\ell\left(\vec{p},\vec{p}';s,\vec{P},\beta\right)=u_\ell\left(\left|\vec{p}-\vec{p}'\right|\right)-(2\pi)^{-2}\int_0^\infty k^2\,d\vec{k}\,u_\ell\left(\left|\vec{p}-\vec{k}\right|\right)$$

$$\times\left[g_0(k,s)Q\left(\vec{k},\vec{P},\beta\right)-g_0^+(k,s)\overline{Q}\left(\vec{k},\vec{P},\beta\right)\right]T_\ell\left(\vec{k},\vec{p}';s,\vec{P},\beta\right). \tag{8}$$

This equation represents the full-off-shell T-matrix pertaining to a relative partial wave ℓ, from which the on-energy-shell counterpart $T_\ell\left(\vec{p},\vec{P}\right)$ is obtained directly by setting $\vec{p}=\vec{p}'$ and $s=p^2$. Clearly, in the free-scattering limit, $Q(\overline{Q})\rightarrow 1(0)$; so that Eq. (2) reduces to the Lippmann-Schwinger t-matrix. The parameterized $T_\ell(p;P;\beta)$ in terms of real effective many-body shifts $\delta_\ell^E(p;P,\beta)$ is:

$$T_\ell(p;P;\beta)=-\frac{2\pi}{p\left(Q(p;P,\beta)+\overline{Q}(p;P,\beta)\right)}\left[\sin\left(2\delta_\ell^E(p;P,\beta)\right)+i\left(1-\cos\left(2\delta_\ell^E(p;P,\beta)\right)\right)\right]; \tag{9}$$

so that, $\delta_\ell^E(p;P,\beta)\equiv\tan^{-1}\dfrac{\mathrm{Im}T_\ell(p;P;\beta)}{\mathrm{Re}T_\ell(p;P;\beta)}$ (10)

General expressions for the total cross section (σ_T), is given by [6]

$$\sigma_T=\frac{8\pi}{k^2}\sum_{\ell(\text{even})}^{\infty}(2\ell+1)\sin^2\left(\delta_\ell^E(k)\right); \tag{11}$$

The above T-matrix takes into account only 'ladder' diagrams; the long-range 'ring' diagrams are not included here, nor is the 'self-energy insertion'. Cumulative experience [8] indicates that this is justified in gaseous, relatively low-dense (in the sense that the interaction range < the interparticle spacing) and weakly-interacting systems, such as ours.

Results and Discussion

The effective Kr-Kr total cross sections were calculated using the HFD-B potential. It was found necessary to include partial waves up to $\ell = 14$ so as to obtain an accuracy to better than ~ 0.5%. Our results are summarized in Figs. 1- 3 and Tables 1-2. In Fig. 1 we plot the computed total cross section and the even ℓ - wave components σ_ℓ ($\ell = 0, 2, 4, 6$), various with the relative momentum k. As seen in the figure, the cross section have a peak at a particular energy. The peaks were refered to as resonances,. The resonances are essentially bound states, but with shorter lifetimes. In other words, they are quasi-bound states. These arise because the repulsive angular-momentum barrier ~ $\frac{\ell(\ell+1)}{r^2}$ 'screens' the short–range repulsive part of the interatomic potential, thereby allowing the interacting particles to 'see' in effect more attraction. At k~0.78 Å^{-1} S-wave ($\ell = 0$) is the most significant partial wave contributing to the total cross section. With increasing k, σ_0 tends to decrease; whereas the contribution of higher ℓ-waves to the scattering decreases. D-wave ($\ell = 2$) scattering for k ~ 0.831 Å^{-1} dominates; so does G-wave ($\ell = 4$) scattering for k ~0.82 Å^{-1}. The I wave ($\ell = 6$)for k ~ 0.815 Å^{-1} scattering dominate. The minimum is evidence for the Ramsauer-Townsend effect [12], which is a physical phenomenon occurring in the collision between two particles when the total cross section is a minimum and, therefore, the mobility is a maximum [2] It appears in electronic systems and in ^{4}He-^{4}He [15] . In the high-energy region, there are undulations in σ_T. These originate from the indistinguishability of Kr atoms, which are scattered by the repulsive part of the potential. [14].

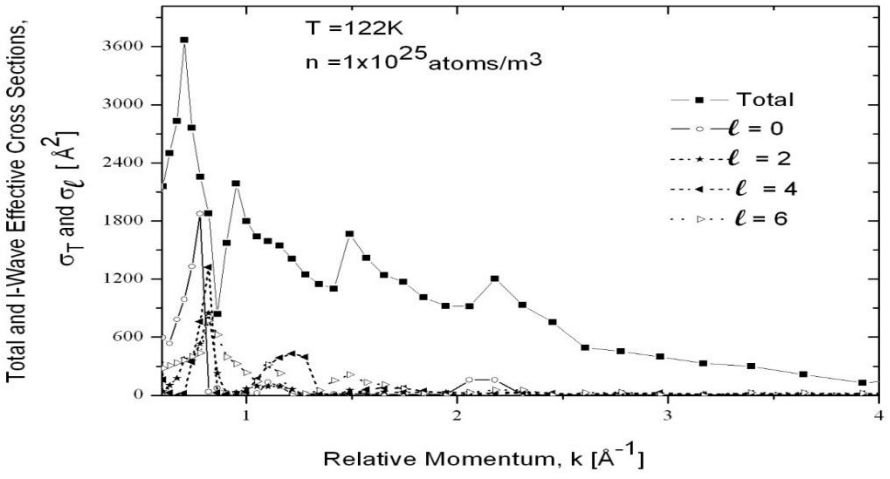

Figure 1: The total cross section σ_T [Å^2], the ℓ-wave effective cross sections σ_ℓ [Å^2], $\ell = 0,2,4,6$ for Kr-Kr scattering varies with the relative momentum k [Å^{-1}] at n=1×10^{25}atoms/m^3.

The energies of all resonances E_R can be determined from $E_R = \left(\frac{\hbar^2 k_R^2}{m} \right)$, k_R being the relative momentum at resonance k_R; they are given in Table 1. On other hand, our results for E_{min} are presented in Table 1.

Table 1: The relative momentum k_R ; $E_R[K]$; k_{min} and $E_{min}[K]$ of the weakly-bound $(Kr)_2$-dimer for various ℓ.

ℓ	k_R [Å^{-1}]	E_R[K]	k_{min} [Å^{-1}]	E_{min}[K]
0	0.78	0.365	0.90	0.486
2	0.831	0.414	1.20	0.864
4	0.82	0.403	0.91	0.497

we saw in Fig.2 that the total cross section hardly dependent on T, but in Fig.3 obviously, the total cross's dependence on n.

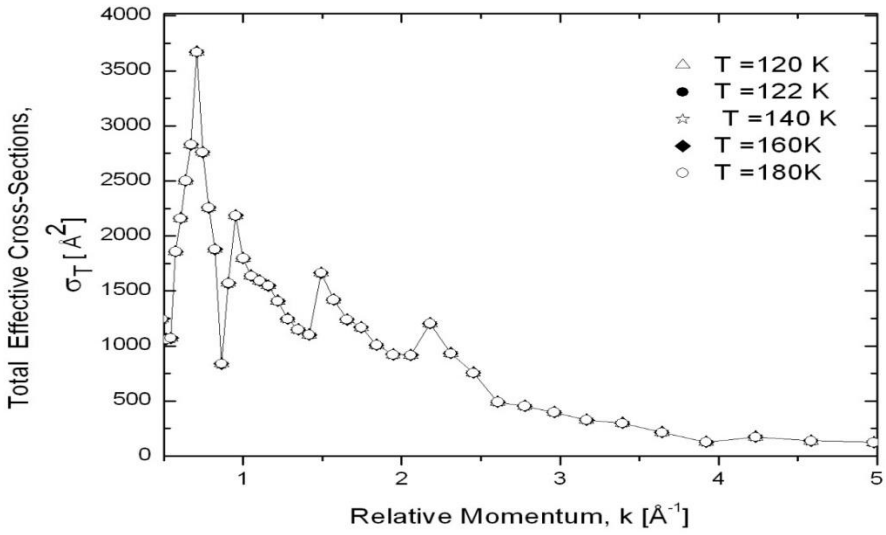

Figure 2: The effective total cross section σ_T [Å^2] for Kr-Kr scattering various with the relative momentum k [Å^{-1}] for different temperatures T [K].

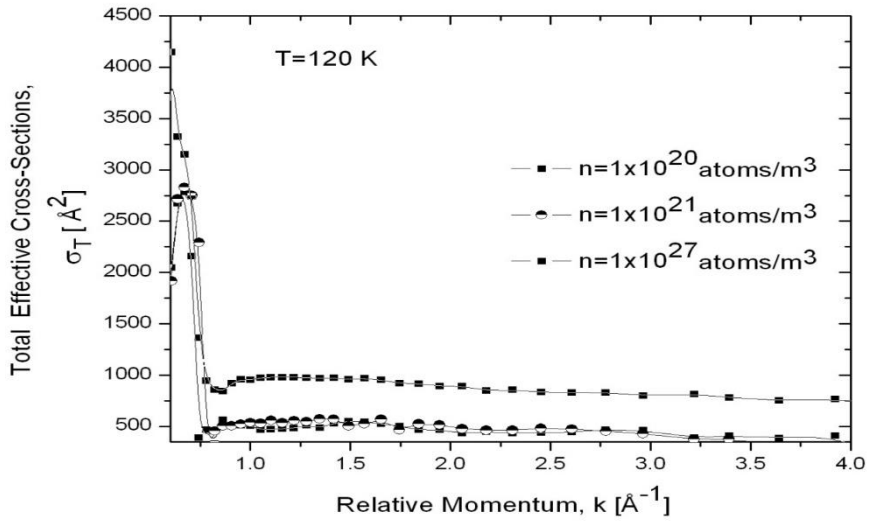

Figure 3: σ_T [Å^2] for Kr-Kr scattering various with k[Å^{-1}] for different n .

To analyze this behavior, the effective scattering length a_o is introduced. This is defined such that $\sigma_T(k) \underset{k\to 0}{\to} 8\pi a_o^2$ [13], where $a_o = -\lim_{k\to 0} \frac{\sin\delta_0}{k}$. (12)

The scattering length has the dimension of length, it is a parameter that represents the strength of the scattering, not its range. The sign the scattering length also, carries physical information: as $k \to 0$, no scattering occurs; $a_o \to 0$ and $\delta_o \to 0$. At k < 2.6 Å^{-1}, corresponding to relatively large interatomic spacing r: the Kr-Kr interaction becomes attractive, $a_o < 0$. At k > 2.6 Å^{-1}, corresponding to relatively small r, the Kr-Kr interaction becomes repulsive, $a_o > 0$. Table 3 exhibits the relation between n and a_0 at different T. It is noted that a_0 and $\sigma_T(0)$ depend on n but hardly on T: at low n, $a_0 < 0$ (attractive case); whereas at high n, $a_0 >> 0$ (weakly-bound, fragile case).

Table 2: The scattering length a_0 [Å] and the total cross section $\sigma_T(0)$ [Å^2] for Kr-Kr at different temperatures T [K] for two different number densities n.

T [K]	n=1×10^{20}atoms/m^3		n=1×10^{27}atoms/m^3	
	a_0 [Å]	$\sigma_T(0)$ [Å^2]	a_0 [Å]	$\sigma_T(0)$ [Å^2]
120	-2.160	117.19	209.10	109.832×10^3

Table 2: (Continued): The scattering length a_0 [Å] and the total cross section $\sigma_T(0)$ [Å^2] for Kr-Kr at different temperatures T [K] for two different number densities n.

124	-2.161	117.30	195.71	96.216×10^3
140	-2.162	117.41	183.28	84.382×10^3
160	-2.163	117.52	171.78	74.250×10^3

Conclusion

In this paper the Galitskii-Migdal Feynman (GMF) formalism, which is essentially an independent-pair model in the presence of a many-body medium, was used for investigating Kr gas at temperature range (120-180K) and at different number density. The total cross section and the even ℓ-wave components σ_ℓ ($\ell = 0, 2, 4, 6$) were computed, we saw that the S-wave is the most significant partial wave contributing to the total cross section. The cross section was observed to have a peak at a particular energy (bound states), these peaks are refered to as resonances. The minimum is evidence for the Ramsauer-Townsend effect when the total cross section is a minimum. In the high-energy region, there are undulations in σ_T. These originate from the indistinguishability of Kr atoms, which are scattered by the repulsive part of the potential. We was computed the energies of all resonances, minimum energy and the scattering length. We plot total cross section versus the relative momentum k at different values of T and different values of n, we noted that the total cross section hardly dependent on T, but the total cross's dependence on n. Repulsive case at k > 2.6 Å^{-1}, such that, $a_o > 0$, (attractive case) at k < 2.6 Å^{-1}where $a_o < 0$.

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Received: December 21, 2017; Published: January 21, 2018