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Author
Miller, William H.

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William H. Miller

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LAWRENCE RADIATION LABORATORY
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DISCLAIMER

MOLECULAR RAMSAUER-TOWNSEND EFFECT IN VERY LOW ENERGY He^4-He^4 SCATTERING*

William H. Miller‡

Inorganic Materials Research Division
Lawrence Radiation Laboratory,
Department of Chemistry,
University of California,
Berkeley, California 94720

ABSTRACT

It is shown that a Ramsauer-Townsend effect is possible in very low energy (~ 2°K) collisions of He^4-He^4 — i.e., a deep minimum in the total elastic scattering cross section occurs at this collision energy. It is seen that no such minimum is possible for the other isotopic variants, He^3-He^3 and He^3-He^4.

I. Introduction

Explanation of the Ramsauer-Townsend (RT) effect in low energy scattering of electrons from rare gas atoms was one of the first successful applications of wave mechanics to collision problems.[1] The physical observation is that at a particular value of the electron collision energy (usually a few tenths of an electron-volt) the total scattering cross section is anomalously small, or equivalently, the mean few path of electrons in the gas is correspondingly large. Electrons at this energy, therefore, propagate through the gas as essentially free, unscattered particles.

In this paper we consider the question of whether such an effect can ever arise in the case of elastic scattering of heavy particles (i.e., atoms and molecules). Since an essential requirement for the effect is that only s-waves ($\ell = 0$ relative orbital angular momentum) contribute significantly to the scattering, the answer at first glance seems to be an obvious "no", for it is well-known that heavy particle scattering typically involves many partial waves.[2] At sufficiently low energy, however, even heavy particle collisions involve only s-wave scattering; these are "very low" energies, typically a few degrees Kelvin.

The next two sections summarize the requirements for a RT effect and consider the restrictions this imposes on an atom-atom system. It is seen that the only molecular system for which it is reasonably possible is He^4-He^4, and the minimum in the cross section occurs at a collision energy ~2°K. Bose statistics plays a crucial role in the existence of the RT effect; i.e., it can not occur for He^3-He^3 or He^3-He^4 collisions.

II. Conditions for a Ramsauer-Townsend Effect.

If the collision energy is sufficiently low, the total elastic scattering cross section is

$$\sigma(E) = 4\pi(\hbar^2/2\mu E)\ \sin^2\eta_o(E), \tag{1}$$

where η_o is the s-wave phase shift, and "sufficiently low" means that the phase shifts for $\ell > 0$ are negligibly small.

Considering a typical atom-atom potential with an attractive well and repulsive wall (e.g., a Lennard-Jones 6-12 potential), the s-wave phase shift at low enough energy is positive due to the fact that only the negative region of the potential is experienced in a low energy collision. At $E = 0$, in fact, $\eta_o = n\pi$, n being the number of s-wave bound states of the diatom. Even if $n = 0$, though, the s-wave phase shift is still positive in the energy region just above zero[3]. Figure 1 sketches the energy dependence of $\eta_o(E)$ for the case that there is one state of the diatom "just barely" bound, compared to the case that the potential is weakened slightly so that the state is "just barely" not bound. In either case the phase shift is positive as $E \to 0$, but becomes negative as E increases and the repulsive wall of the potential begins to make a greater contribution to the phase shift than the attractive region.

It is clear, therefore, that there is an energy E_o at which the s-wave phase shift is zero; Equation (1) then gives a zero cross section, meaning that only higher partial waves contribute. If E_o is so small that these higher partial waves have not begun to contribute significantly, then the cross section at E_o is anomalously small, and this is the RT effect.

Finally, one should note that η_o need not actually be zero at E_o, but an integer multiple of π; i.e., the arguments above are unchanged if one re-labels Figure 1 so that π becomed $n\pi$, and zero becomes $(n-1)\pi$.

III. WKB Analysis for a Lennard-Jones Potential.

One might question the validity of using the WKB approximation to describe phase shifts in this low energy region. Even at E = 0, however, although η_o^{WKB} is not an integer multiple of π, it is a reasonably good approximation to $n_o\pi$; this is actually a good way to estimate the number of bound states in a given potential.[4] The WKB phase shift will not show the bending over as the dotted line in Figure 1, but it will be roughly correct for energies as large as E_o.

For purposes of estimating the requirements for an atom-atom collision system to demonstrate a RT effect, consider a Lennard-Jones 6-12 potential,

$$V(r) = 4\epsilon[(\sigma/r)^{12} - (\sigma/r)^{6}] . \qquad (2)$$

The WKB approximation gives the s-wave phase shift as

$$\eta_o(E) = Df(\lambda), \qquad (3)$$

where $\lambda = E/\epsilon$, $D = \sigma(2\mu\epsilon)^{1/2}/\hbar$, and f is the following universal function of λ:

$$f(\lambda) = \int_0^{\alpha} dx[(\alpha-x)(\beta+x)]^{-1/2}(x^{-1/6}-2x^{5/6}) \qquad (4)$$

$$\alpha = [1 + (1+\lambda)^{1/2}]/2$$

$$\beta = [-1 + (1+\lambda)^{1/2}]/2 ;$$

f can be expressed in terms of hypergeometric functions. For small λ one has

$$f(\lambda) \simeq a - b\lambda^{1/3} \qquad (5)$$

where

$$a = \Gamma(4/3)\ \Gamma(3/2)/\Gamma(11/6) \simeq 0.8413$$
$$b = 3.2^{-2/3}\ \Gamma(5/6)\ \Gamma(2/3)/\Gamma(1/2) \simeq 1.6298.$$

Thus f has a zero at λ_o,

$$\lambda_o \simeq (a/b)^3 = 0.138;$$

solving for the root numerically [without the approximation in Equation (5)], one finds $\lambda_o = 0.140$.

For $E = E_o (E_o \equiv \lambda_o \epsilon \simeq .14\epsilon)$, therefore, the s-wave phase shift vanishes, so that the magnitude of the cross section at E_o is determined by the next highest partial wave; normally this is $\ell = 1$, but if the atoms are identical bosons, odd values of ℓ are not allowed,[5] so that $\ell = 2$ gives the first non-zero phase shift.

The magnitude of the first non-zero phase shift ($\ell = 1$ or 2) can be estimated by the "large ℓ" limit of the WKB phase shift (the Jeffreys-Born, or Eikonal approximation). Although ℓ is obviously not "large", the approximation actually depends on the inequality

$$V(r) \ll \frac{\hbar^2 \ell^2}{2\mu r^2},$$

for all $r > \ell/k$; for low enough energy, therefore, this inequality is fulfilled. for any $\ell > 0$. Since only large values of r are involved, one only needs to consider the long-range attractive part of the potential, and obtains

$$\eta_{\ell}(E) = (3\pi/8)\, D^6 \lambda^2 \ell^5 \ , \tag{6}$$

where one actually makes the replacement $\ell \to [\ell(\ell+1)]^{1/2}$, or $(\ell + 1/2)$, and $\ell = 1$ or 2. At E_o, therefore, the magnitude of the cross section is

$$\sigma(E_o) \simeq 4\pi(1 + \delta_{\ell,2})(2\ell+1)[\eta_{\ell}(E_o)]^2$$

and with Equation (6) this is

$$\sigma(E_o) \simeq \pi\sigma^2(1 + \delta_{\ell,2})(9\pi^2/8)D^{10}\lambda_o^{\ 3}(\ell + 1/2)^{-9}, \tag{7}$$

with $\ell = 1$ or 2.

The RT effect is significant if $\sigma(E_o)$ is much smaller than $\pi\sigma^2$ (the "hard sphere" cross section). Since λ_o and ℓ are fixed values, this will be true if D is sufficiently small — i.e., it is the value of D which determines the extent of the RT effect. The fact that $\sigma(E_o)$ in Equation (7) is proportional to D to such a high power means that the cut-off value of D — that value below which the RT effect is prominent and above which it is non-existent — is quite sharp. If one supposes that $\sigma(E_o)$ must be below $.1\pi\sigma^2$ for the RT effect to be significant, Equation (7) gives $D_1 = 1.62$ for $\ell = 1$ and $D_2 = 2.40$ for $\ell = 2$ as these cut-off values. For values of D less (greater) than D_1 or D_2, there should (should not) be a significant RT effect.

The above discussion has considered the situation that there are no (or just barely one) $\ell = 0$ bound states in the two-body potential. The arguments may be modified to handle the more general situation, but this hardly seems warranted — if the potential is this strongly attractive, a collection of the particles will probably be a solid at temperatures low enough for these considerations to be of interest.

IV. Helium-Helium Collisions.

The D parameter for most atom-atom systems is much larger than the critical values obtained above. For the interaction of two helium atoms, however, one has[6] $\epsilon \simeq 8.94 \times 10^{-4}$ eV and $\sigma \simeq 2.64$ Å, so that $D \simeq 2.46$ for He^4-He^4, and $D \simeq 2.28$ for He^3-He^4; s-waves cannot contribute to He^3-He^3 scattering,[5] so no RT effect is possible here. Since $\ell = 1$ contributes for He^3-He^4 and $D_1 \simeq 1.62$ is the maximum value of D for which the RT effect is estimated to be significant, one concludes that there is definitely not a RT effect in He^3-He^4 scattering.

For He^4-He^4, however, $\ell = 2$ is the first term past $\ell = 0$, and since it is estimated that the RT effect should be significant for values of D up to $D_2 \simeq 2.40$, the value $D \simeq 2.46$ for He^4-He^4 makes this a borderline case. One expects there to be some evidence of the RT effect, but just how deep the minimum in the cross section at E_0 is depends in a sensitive way on the precise shape of the outer wall of the potential well.

Several recent quantum calculations[7,8] of He^4-He^4 total elastic cross sections at very low energies have shown this RT minimum. With $\epsilon \simeq 10°$K the WKB treatment of Section III predicts the minimum at $E_0 \simeq 1.4°$K, whereas these quantum calculations find it at $\sim 1.8°$K. Figure 5 of Dondi et al[7] shows dramatically how sensitive to the shape of the potential is the depth of the RT minimum, ranging from below 20 Å^2 to over 100 Å^2 for various potentials all with the same ϵ and r_m.

In conclusion, it is seen that there is the possibility of a prominent RT minimum in the two-body scattering cross section of He^4-He^4 at a collision energy ~ 2°K; there is no such possibility for He^3-He^3 or He^3-He^4 collisions. If such a "window" exists in the two-body cross section, it is interesting to speculate whether or not it in any way enhances the peculiar properties of He^4 in this temperature range.

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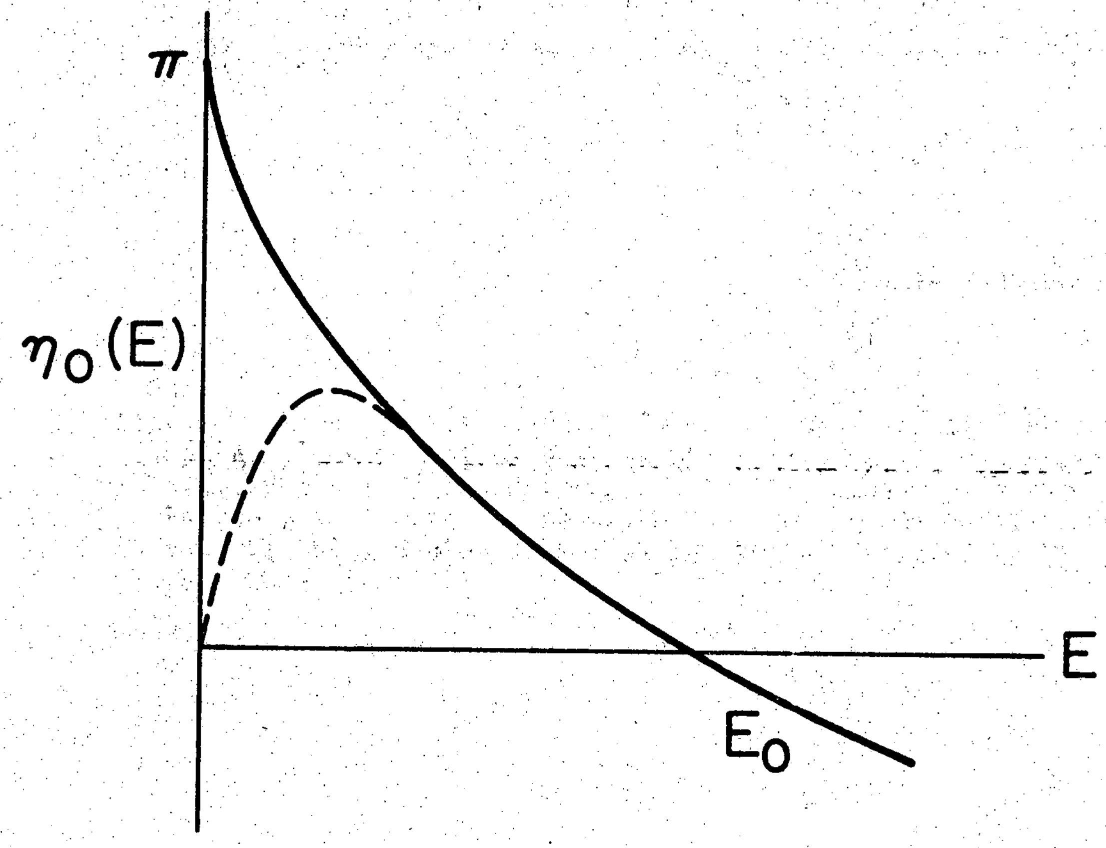

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Fig. 1. Sketch of the s-wave phase shift as a function of collision energy for a potential with an attractive well and a repulsive wall; the solid line corresponds to the situation in which there is one bound state in the potential, and the dashed line corresponds to a slightly weaker potential for which the state is "just barely" not bound.

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LAWRENCE RADIATION LABORATORY
UNIVERSITY OF CALIFORNIA
BERKELEY, CALIFORNIA 94720