Calculation of the scattering length in atomic collisions using the semiclassical approximation

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A simple analytical formula, $a = \bar{a}\,[1 - \tan\frac{\pi}{n-2}\tan(\Phi - \frac{\pi}{2(n-2)})]$, is obtained for the scattering length in atomic collisions. Here $\bar{a} = \cos[\pi/(n-2)]\,\{\sqrt{2M\alpha}/[\hbar(n-2)]\}^{2/(n-2)}\,\Gamma(\frac{n-3}{n-2})/(\Gamma\frac{n-1}{n-2})$ is the mean scattering length determined by the asymptotic behavior of the potential $U(r) \sim -\alpha/R^n$ ($n = 6$ for atom-atom scattering or $n = 4$ for ion-atom scattering), M is the reduced mass of the atoms, and Φ is the semiclassical phase calculated at zero energy from the classical turning point to infinity. The value of $\bar{a}$, the average scattering length, also determines the slope of the s-wave phase shifts beyond the near-threshold region. The formula is applicable to the collisions of atoms cooled down in traps, where the scattering length determines the character of the atom-atom interaction. Our calculation shows that repulsion between atoms ($a > 0$) is more likely than attraction with a "probability" of 75%. For the Cs-Cs scattering in the $^3\Sigma_u$ state, $\bar{a} = 95.5a_B$ has been obtained, where a_B is the Bohr radius. The comparison of the calculated cross-section energy dependence with the experimental data gives evidence for a positive value for the Cs-Cs scattering length, which makes cesium Bose gas stable.

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I. INTRODUCTION

In the past few years great progress was made in experiments with atoms in traps. The combination of laser and evaporative cooling and magnetic traps enabled the production of gases with spin-aligned atoms at extremely low temperatures together with relatively large densities. For instance, the best values of [1] for Cs are $T \sim 1\ \mu$K, $n \sim 10^{10}$ cm^{-3}, and in the experiments with hydrogen atoms [2] the values of $T \sim 100\ \mu$K, $n \sim 8\times10^{13}$ cm^{-3} have been achieved. These conditions bring the samples towards the Bose-Einstein-condensation (BEC) point, and the character of the interaction of atoms should be of crucial importance for the behavior of the system in the near-critical conditions.

As is known, the collisional properties of particles at low energies are determined by the s-wave scattering, and expressed in terms of one parameter—the scattering length a. It determines the behavior of the s-wave phase shift δ_0 and the scattering cross section σ (see, e.g., [3]):

$$\delta_0 = -ak\ , \qquad \sigma = 4\pi a^2, \qquad (1)$$

where k is the relative wave vector of the colliding particles. The formulas (1) are valid for $ak < 1$. If the scattering length is not abnormally small, and the scattering in higher partial waves does not display any peculiar low-lying resonances, we can neglect their contribution to the cross section for all $k < a^{-1}$, or more precisely, $k \ll a^{-1}$. At temperatures obtained in the experiments [1,2] the thermal values of the atomic momenta, $p \sim \sqrt{2mkT}$, are very small. The corresponding magnitude of the wave vector $k = p/\hbar$ is nearly the same for both types of atoms:

$k \sim 10^{-3}a_B^{-1}$ (a_B is the Bohr radius). Therefore, the approximation (1) is already valid for H and Cs gases if $a \ll 10^3 a_B$, which seems quite plausible.

The actual value of the scattering length is determined by the potential energy $U(R)$ of interatomic interaction. In the case of hydrogen or cesium atoms in a magnetic trap the spins of the atoms are parallel. Thus, the potential curve refers to the $^3\Sigma_u$ state of the atomic pair. At large distances $U(R)$ falls off as

$$U(R) \simeq -\frac{\alpha}{R^n}, \qquad (2)$$

where $n = 6$ for neutral atoms with $J = \frac{1}{2}$ ground state (*van der Waals* forces), or $n = 4$ for the ion-atom interaction. At smaller distances the attraction is replaced by strong electron-exchange repulsion, which increases exponentially. The net action of both forces produces a potential well (see the sketch in Fig. 1), which fixes the magnitude and the sign of the scattering length. The sign of a determines whether atoms are repulsed ($a > 0$) or attracted ($a < 0$) at very low temperatures.

On the whole the $^3\Sigma_u$ potential curves are well known for hydrogen [4], and known with less certainty for cesium [5,6] atoms. The depth of the potential well $U_{\min}$ and the position of the minimum $R_{\min}$ are the following. For H$_2$: $U_{\min} = -0.20 \times 10^{-4}$ a.u., $R_{\min} = 7.9a_B$, and for Cs$_2$: $U_{\min} \simeq -1.3 \times 10^{-3}$ a.u., $R_{\min} \simeq 12a_B$. Throughout the paper we will use the atomic units, in which $a_B = 1$, and the atomic masses are $m_H = 1836$ a.u. and $m_{Cs} = 2.422 \times 10^5$ a.u.

The strength of the potential $U(R)$ may be characterized by the dimensionless parameter $Mb^2|U_0|/\hbar^2$, where M is the reduced mass of the atomic pair and b and U_0 are the typical radius and depth of the potential. Using

$U_0 \sim |U_{\min}|$ and $b \sim R_{\min}$, one obtains for the strength of the $^3\Sigma_u$ potential the value of 1.1 for hydrogen and 2×10^5 for cesium. It means that for hydrogen the potential is weak, and there are no bound states for $H_2\,{}^3\Sigma_u$. The scattering length for triplet hydrogen-hydrogen scattering is of the order of the atomic size $a = 1.36$ a.u. [7]. It is positive, which means that low-energy spin-aligned hydrogen atoms interact repulsively despite the attractive long-range van der Waals forces.

In the case of the Cs-Cs pair the potential is very deep. Our calculations show (see Sec. III) that it produces more than 50 bound $^3\Sigma_u$ states. Therefore the wave function of the scattering atoms repeatedly oscillates within the potential well. It means that any minor uncertainty in the shape of the potential can easily produce noticeable changes in the asymptotic behavior of the wave function, and consequently change the phase shift and the scattering length.

On the other hand, the smallness of the wavelength in comparison with the typical radial scale of the potential variation naturally suggests the use of the semiclassical approximation. The latter has enabled us to show (Sec. II) that the scattering length for the potential of this type with can be expressed in the following way:

$$a = \bar{a}\left[1 - \tan\left(\tfrac{\pi}{n-2}\right)\tan(\Phi - \xi)\right]. \tag{3}$$

Here

$$\bar{a} = \cos\left(\frac{\pi}{n-2}\right)\left(\frac{\sqrt{2M\alpha}}{\hbar(n-2)}\right)^{\frac{2}{n-2}} \Gamma\left(\frac{n-3}{n-2}\right)\Big/\Gamma\left(\frac{n-1}{n-2}\right)$$

is the mean scattering length. It is solely determined by the asymptotic behavior (2) of the potential. Φ is the semiclassical phase calculated at zero energy from the classical turning point to infinity, and ξ is a small phase addition, which depends on the boundary condition at the turning point. The dependence of $\bar{a}$ on the parameters of the potential is smooth. On the contrary, when the phase is large, $\Phi \gg 1$ (e.g., for cesium $\Phi \sim 180$), it follows from (3) that the scattering length oscillates around the positive value of $\bar{a}$, with a "probability" of $\frac{n-3}{n-2}$ being positive, and of $\frac{1}{n-2}$ being negative (for neutral atoms with $n = 6$: 75% and 25%, respectively). For Cs ($\alpha = 7020$ a.u., [8]) we obtain $\bar{a} \simeq 100$ a.u.

Using the appropriate analytical approximation for the $Cs_2\,{}^3\Sigma_u$ potential, we calculated the s-wave phase shift for k values up to $0.05a_B^{-1}$, and studied the dependence of the phase shift and the scattering length upon the small variations of the fitting parameter of the potential (Sec. III). The values of the scattering length obtained by the numerical solution of the Schrödinger equation agree well with those calculated from (3). It is shown that the positive value of $a \simeq 70$ a.u. is consistent with recent measurements of the elastic Cs-Cs scattering cross section in the range of temperatures from 30 to 250 μK [9]. The negative a value contradicts the experimental data.

In the conclusion (Sec. IV) we consider some possible generalizations of the results obtained in the paper, and their applications to the BEC.

II. CALCULATION OF THE SCATTERING LENGTH

A. Scattering length in the semiclassical approximation

Let us now proceed to the calculation of the scattering length. It will be obtained by matching the semiclassical wave function inside the potential well with the exact solution in the asymptotic region (2). A typical potential curve $U(R)$ for the atom-atom interaction is shown in Fig. 1. In order to find the scattering length a it is necessary to solve the radial Schrödinger equation for the s partial wave at zero energy:

$$-\frac{\hbar^2}{2M}\frac{d^2\chi(R)}{dR^2} + U(R)\chi(R) = 0 \tag{4}$$

with the boundary condition $\chi(0) = 0$. Then a can be found from the asymptotic behavior of $\chi(R)$ at large distances:

$$\chi(R) \underset{R\to\infty}{\sim} C_1 R + C_2 \tag{5}$$

and

$$a = -\frac{C_2}{C_1}. \tag{6}$$

We shall suppose that within the potential well the semiclassical (WKB) approximation is valid. It implies the fulfillment of the following conditions:

$$\left|\frac{d\lambda}{dR}\right| \ll 2\pi \quad \text{or} \quad \frac{M\hbar|F|}{p^3} \ll 1. \tag{7}$$

Here λ is the de Broglie wavelength, $p = \sqrt{2M[-U(R)]}$ is the local momentum of the particle at zero energy, and $F = -dU/dR$ is the force acting upon the particle. As usual, the condition (7) is violated in the vicinity of the classical turning point R_0, where $p = 0$ (see Fig. 1). To the right of the turning point the solution is [3]

$$\chi(R) = \frac{C}{\sqrt{p}}\cos\left(\frac{1}{\hbar}\int_{R_0}^{R} p\,dR - \frac{\pi}{4}\right), \quad R > R_0, \tag{8}$$
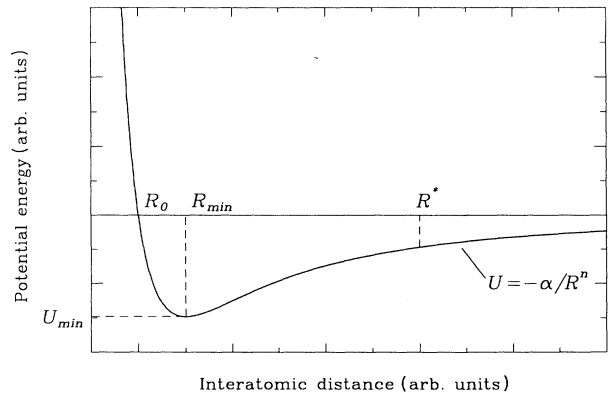

FIG. 1. The typical interatomic potential and characteristic values of R.

whereas to the left of R_0 $\chi(R)$ decreases exponentially.

At large distances the potential decreases as $-\alpha/R^n$, and we can check condition (7) explicitly. It yields

$$R \ll \left(\frac{2\gamma}{n}\right)^{\frac{2}{n-2}} , \qquad (9)$$

where

$$\gamma = \frac{\sqrt{2M\alpha}}{\hbar} . \qquad (10)$$

Thus, the WKB approximation is violated at large distances. This can be also seen from the fact that (8) fails to reproduce the asymptotic behavior (5): when $R \to \infty$ $\chi(R) \propto p^{-\frac{1}{2}} \cos(\text{const}) \propto R^{\frac{n}{4}}$.

However, if γ is large enough the semiclassical solution (8) can be used up to distances where the asymptotic expression (2) for $U(R)$ is valid, and where the equation (4) turns into

$$\chi''(R) + \frac{\gamma^2}{R^n}\chi(R) = 0 . \qquad (11)$$

Indeed, the estimation of the right-hand side of (9) for Cs ($\gamma = 4.12 \times 10^4$) gives the value of 117 a.u., whereas the potential curve turns into its asymptotic R^{-6} drop at much smaller distances. Hence, we can always find the radius R^*, at which both the WKB solution and Eq. (11) are valid (see Fig. 1).

Introducing the new function φ, $\chi = \varphi\sqrt{R}$, and the new variable x, $R = \left(\frac{2\gamma}{(n-2)x}\right)^{\frac{2}{n-2}}$, Eq. (11) is transformed into the Bessel equation:

$$\frac{d^2\varphi}{dx^2} + \frac{1}{x}\frac{d\varphi}{dx} + \left[1 - \frac{1}{(n-2)^2 x^2}\right]\varphi = 0 . \qquad (12)$$

The arbitrary solution of (12) is represented by a linear combination of Bessel and Neumann functions $J_{\frac{1}{n-2}}(x)$ and $N_{\frac{1}{n-2}}(x)$. Therefore, in the range of $R > R^*$ the solution of Eq. (4) is

$$\chi_>(R) = \sqrt{R}\left[A\, J_{\frac{1}{n-2}}\left(\frac{2\gamma}{n-2}R^{-\frac{n-2}{2}}\right)\right.$$
$$\left. -B\, N_{\frac{1}{n-2}}\left(\frac{2\gamma}{n-2}R^{-\frac{n-2}{2}}\right)\right] . \qquad (13)$$

Using the expansions for the Bessel and Neumann functions for $x \ll 1$ $(R \to \infty)$ and keeping the lower-order terms,

$$J_\nu(x) \simeq \frac{x^\nu}{2^\nu\Gamma(1+\nu)} ,$$

$$N_\nu(x) \simeq \cot(\pi\nu)\frac{x^\nu}{2^\nu\Gamma(1+\nu)} - \frac{1}{\sin\pi\nu}\frac{x^{-\nu}}{2^{-\nu}\Gamma(1-\nu)} ,$$

one obtains from (13) the necessary linear asymptotic behavior of the type (5) for $\chi_>(R)$, with a scattering length (6) given by

$$a = \cos\left(\frac{\pi}{n-2}\right)\left(\frac{\gamma}{n-2}\right)^{-\frac{2}{n-2}}\frac{\Gamma(\frac{n-3}{n-2})}{\Gamma(\frac{n-1}{n-2})}$$
$$\times\left[1 - \frac{A}{B}\tan\frac{\pi}{n-2}\right] . \qquad (14)$$

The constants A and B are obtained by matching the analytical solution (13) to the WKB wave function (8) at $R = R^*$. Since R^* has been chosen to satisfy the condition (9), the value of the argument x of the cylindrical functions corresponding to the point R^* is large: $x = \frac{2\gamma}{n-2}R^{*-\frac{n-2}{2}} \gg 1$. Thus, we can use the asymptotic formulas for $J_\nu(x)$ and $N_\nu(x)$ at $x \gg 1$, so that (13) turns into

$$\chi_>(R) = \sqrt{\frac{n-2}{\pi\gamma}}\, R^{\frac{n}{2}}\left\{\left(A - B\cot\frac{\pi}{n-2}\right)\cos\left(\frac{2\gamma}{n-2}R^{-\frac{n-2}{2}} - \frac{\pi}{2(n-2)} - \frac{\pi}{4}\right)\right.$$
$$\left. + \frac{B}{\sin\frac{\pi}{n-2}}\cos\left(\frac{2\gamma}{n-2}R^{-\frac{n-2}{2}} + \frac{\pi}{2(n-2)} - \frac{\pi}{4}\right)\right\} \quad (R \simeq R^*). \qquad (15)$$

Calculating the logarithmic derivatives $\chi^{-1}d\chi(R)/dR$ for (15) and (8), and taking into account that when $R \to R^*-$ we can use $U(R) = -\alpha/R^n$ in p and dp/dR, we find the A/B ratio:

$$\frac{A}{B} = \tan\left(\Phi - \frac{\pi}{2(n-2)}\right) , \qquad (16)$$

where $\Phi = \Phi_< + \Phi_>$ and the phases $\Phi_{<,>}$ are

$$\Phi_< = \frac{1}{\hbar}\int_{R_0}^{R^*} p\,dR , \quad \Phi_> = \frac{2\gamma}{n-2}R^{*-\frac{n-2}{2}} .$$

The second equation is just the addition to the semiclassical phase from the distances of R^* to ∞:

$$\Phi_> = \frac{2\gamma}{n-2}R^{*-\frac{n-2}{2}} = \frac{1}{\hbar}\int_{R^*}^{\infty}\sqrt{2M\frac{\alpha}{R^n}}dR . \qquad (17)$$

Therefore we see that the sum Φ is the semiclassical phase calculated at zero energy from the classical turning point to infinity, and its magnitude does not depend on the matching radius R^*. It is also worth noting here that the condition (9) for the validity of the WKB approximation for the $-\alpha/R^n$ potential is equivalent to the requirement that the contribution to the semiclassical phase from the asymptotic region $R > R^*$ should be large: $\Phi_> \gg 1$.

Introducing now the A/B ratio (16) into (14), we arrive at the final formula for the scattering length:

$$a = \cos\left(\frac{\pi}{n-2}\right)\left(\frac{\gamma}{n-2}\right)^{\frac{-2}{n-2}}\frac{\Gamma(\frac{n-3}{n-2})}{\Gamma(\frac{n-1}{n-2})}$$

$$\times\left[1 - \tan\frac{\pi}{n-2}\tan\left(\Phi - \frac{\pi}{2(n-2)}\right)\right] \qquad (18)$$

where

$$\Phi = \frac{1}{\hbar}\int_{R_0}^{\infty}\sqrt{2M[-U(R)]}dR \ . \qquad (19)$$

This result has the structure of (3). The factor before the square brackets depends only on the parameters α and n of the asymptotic behavior (2) of the potential, and the reduced mass M of the scattering particle [see the definition of γ (10)]. It represents a kind of mean, characteristic scattering length $\bar{a}$, which slowly varies with the parameters of the potential well.

The semiclassical phase Φ (19) determines the actual magnitude of the scattering length (18). Calculating the integral (19) with a finite upper limit $R_{\max}$ and investigating the convergence of Φ when $R_{\max} \to \infty$, one can find out what range of distances is important for the scattering problem. Roughly speaking, it should be that $R_{\max} \gg \bar{a} \sim \left(\frac{\gamma}{n-2}\right)^{\frac{2}{n-2}}$. If Φ satisfies the condition

$$\Phi - \frac{\pi}{2(n-2)} = \frac{\pi}{2} + \pi N, \qquad N = 1, 2, 3, \ldots, \qquad (20)$$

then the tan( ) and the scattering length (18) go to infinity. It corresponds to the appearence of the Nth bound state in the well.

The behavior of a and $\bar{a}$ as functions of Φ is illustrated in Fig. 2 for the case of $n = 6$ and asuming that $\gamma \propto \Phi$, which seems plausible, if the contribution of $\Phi_>$ (17) to Φ is large. In this case we obtain that $\bar{a} \propto \Phi^{\frac{1}{2}}$. It is clear from Fig. 2 that the scattering length is on the whole more often positive than negative. The measure of Φ intervals in which $a > 0$ is $n - 3$ times larger than that where $a < 0$.

Formula (18) reveals some of the peculiarities of the scattering lengths for the potentials with different n asymptotic behavior. In agreement with the well-known
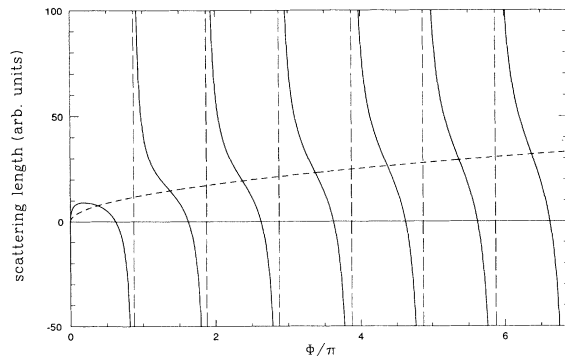

FIG. 2. The dependence of the mean scattering length $\bar{a}$ (short-dashed curve) and the scattering length a (solid curve) on the semiclassical phase Φ.

fact that the constant cross-section limit (1) at zero energy is valid only for the potentials falling off faster than $1/R^3$ (see [3]), the scattering length a goes to infinity when $n \to 3+$.

The other interesting case is $n = 4$. A potential of this type acts between a charged particle and a neutral polarizable one, e.g., between an ion (or electron) and an atom: $U(R) = -\frac{1}{2}\alpha_d e^2/R^4$, $(R \gg a_B)$, where α_d is the atomic dipole polarizability. For $n \to 4$ (18) turns into

$$a = \gamma\tan\left(\Phi - \frac{\pi}{4}\right) = \frac{\sqrt{M\alpha_d e^2}}{\hbar}\tan\left(\Phi - \frac{\pi}{4}\right).$$

Therefore, negative and positive values of a are equally probable for this case. Indeed, due to the polarization potential the electron-atom scattering length often becomes negative. This effect gives rise to the well-known Ramsauer minimum in the scattering cross section.

B. Exactly solvable examples

In this section we would like to illustrate the behavior of the scattering length, using two exactly solvable potentials, and to show that it again "prefers" positive values.

1. Hard core plus $1/R^n$

Let the potential be of the form

$$U(R) = \begin{cases} \infty, & R < R_0 \\ -\alpha/R^n, & R > R_0. \end{cases} \qquad (21)$$

The wave function at zero energy is given by (13) for all $R > R_0$. The boundary condition is now $\chi(R_0) = 0$. It yields for the A/B ratio

$$\frac{A}{B} = \frac{N_{\frac{1}{n-2}}\left(\frac{2\gamma}{n-2}R_0^{-\frac{n-2}{2}}\right)}{J_{\frac{1}{n-2}}\left(\frac{2\gamma}{n-2}R_0^{-\frac{n-2}{2}}\right)}. \qquad (22)$$

Introducing it into (14) we obtain the exact scattering length for (21).

Provided the potential is deep enough, and the argument of the Bessel and Neumann functions is large, $\frac{2\gamma}{n-2}R_0^{-\frac{n-2}{2}} \gg 1$, we can use the asymptotic formulas for J_ν and N_ν in (22). The result then is given by the formula

$$a = \cos\left(\frac{\pi}{n-2}\right)\left(\frac{\gamma}{n-2}\right)^{\frac{-2}{n-2}}\frac{\Gamma(\frac{n-3}{n-2})}{\Gamma(\frac{n-1}{n-2})}$$

$$\times\left[1 - \tan\frac{\pi}{n-2}\tan\left(\Phi - \frac{\pi n}{4(n-2)}\right)\right], \qquad (23)$$

where $\Phi = \frac{2\gamma}{n-2}R_0^{-\frac{n-2}{2}}$ is the analytically calculated phase (19). The only difference between (23) and the general formula for a (18) is the additional $-\frac{\pi}{4}$ phase

shift, which is due to the different boundary conditions at $R = R_0$.

It is interesting to compare the scattering length for the potential with $-\alpha/R^n$ long-range attraction to that for the totally *repulsive* potential: $U(R) = \alpha/R^n$. The scattering length for the latter is always positive (see [3], Sec. 130):

$$a_r = \left(\frac{\gamma}{n-2}\right)^{\frac{-2}{n-2}} \frac{\Gamma(\frac{n-3}{n-2})}{\Gamma(\frac{n-1}{n-2})} ,$$

and it has nearly the same magnitude as the mean scattering length: $\bar{a} = \cos\left(\frac{\pi}{n-2}\right) a_r$.

2. Hard core plus square well

The simplest potential modeling the "hard core plus attraction" interaction can be of the form

$$U(R) = \begin{cases} \infty , & R < R_0 \\ -U_0 , & R_0 \leq R \leq R_1 \\ 0 , & R > R_1. \end{cases}$$

The zero energy s-wave function for it is constructed of $\sin k(R - R_0)$ between R_0 and R_1, and the linear function (5), smoothly joined to it at $R = R_1$. The scattering length is given by

$$a = R_1 \left[1 - \frac{\tan\Phi}{kR_1} \right] , \quad (24)$$

where

$$\Phi = k(R_1 - R_0) \quad \text{and} \quad k = \frac{\sqrt{2MU_0}}{\hbar} .$$

In this model the mean scattering length is given by the outer radius of the well, $\bar{a} = R_1$, and the contribution of the alternating $\tan\Phi$ term in the square brackets is suppressed by the $1/kR_1$ factor. At this point the square well model differs from the potentials with an $1/R^n$ asymptotic behavior, where the contribution of the phase-dependent tangent is regulated by $\tan\frac{\pi}{n-2}$, independently of the potential strength.

III. NUMERICAL RESULTS

In order to perform numerical calculations for the s-wave scattering phase shifts and the scattering length we adopt the following expression for the Cs$_2$ $^3\Sigma_u$ potential curve:

$$U(R) = \tfrac{1}{2}BR^\alpha e^{-\beta R} - \left(\frac{C_6}{R^6} + \frac{C_8}{R^8} + \frac{C_{10}}{R^{10}}\right) f_c(R) . \quad (25)$$

Here the first item on the right-hand side represents the exchange repulsion between valence electrons, and the second one is the sum of van der Waals terms, multiplied by the relevant cutoff function $f_c(R)$ to cancel $1/R^n$ divergence at small distances. The values of the parame-

TABLE I. Parameters for $^3\Sigma_u$ potential curves for H$_2$ and Cs$_2$.

Atoms	B^a	α	β	C_6	C_8	C_{10}
H$_2$	1.65	2.5	2	6.5	124.4	3.29×10^3
Cs$_2$	0.0016	5.53	1.072	7020	1.1×10^6	1.7×10^8

^{a}The values of the parameters are given in atomic units.

ters B, α, β, C_i for the potential (25) were taken from [8] (see Table I). When R tends to zero the exchange term displays erroneous decreasing behavior. However, this range of R does not influence the calculations at all, since the wave function rapidly vanishes to the left of the classical turning point.

The cutoff function is analogous to that used for the H-H $^3\Sigma_u$ potential [7]:

$$f_c(R) = \Theta(R - R_c) + \Theta(R_c - R) \, e^{-(R_c/R - 1)^2} , \quad (26)$$

where $\Theta(x)$ is the unit step function: $\Theta(x) = 1$ (0), when $x > (<) 0$. Therefore, the only free parameter for the potential $U(R)$ (25) is the *cutoff radius* R_c, governing the decrease of the function $f_c(R)$ at $R < R_c$.

The magnitude of the cutoff parameter R_c was adjusted by comparing (25) to the Cs$_2$ $^3\Sigma_u$ potential curve, calculated *ab initio* by Krauss and Stevens [5] from $R = 7$ to 20 a.u. The best fit to the values of $R_{\min}$ and $U_{\min}$ of the potential was obtained for $R_c = 23.165$. Both potential curves are shown in Fig. 3, together with the asymptotic potential of [6]. The latter was calculated by changing the sign of the exchange potential for the $^1\Sigma_g$ curve. Though the values of C_i used in [6] are slightly different from those in Table I, the asymptotic behavior of the curves at $R > 18$ is very close. We have also checked the shape of the potential near $R_{\min}$ by calculating the harmonic vibration frequency ω. Our value of $\omega = 11.2$ cm^{-1} is in good agreement with that of [6], 11 cm^{-1}, and is noticeably less than the frequency of [5]:
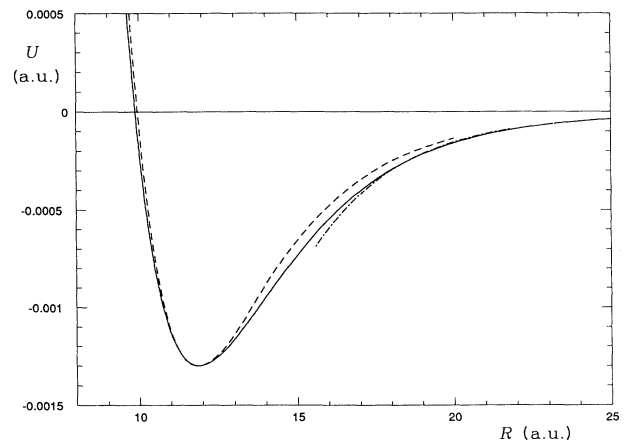

FIG. 3. The Cs$_2$ $^3\Sigma_u$ potential curves: dashed curve, *ab initio* calculation [5]; dot-dashed curve, experimental fit for Cs$_2$ $^1\Sigma_g$ [6] with exchange potential inverted; solid curve, analytical fit (25) for $R_c = 23.165$ a.u.

$\omega = 12.29$ cm^{-1}. Since the potential curve (25) can by no means be treated as an exact one, we have studied the s-wave scattering using different values of R_c around 23.165 a.u.

The potential $U(R)$ for a given R_c value was introduced into the radial s-wave Schrödinger equation. It was solved numerically for a number of positive energies $E = \frac{k^2\hbar^2}{2M}$. The phase shifts $\delta_0(k)$ were obtained from the asymptotic behavior of the wave function: $\chi(R) \propto \sin[kR + \delta_0(k)]$, using the algorithm of [10]. It calculates the total phase of the wave function from $R = 0$ to large R, and derives the phase shift as the difference between the total phase and kR when $R \to \infty$. This procedure eliminates the usual modπ ambiguity in the definition of δ_0, and readily enables to determine the number of bound states in the potential well (see below).

The dependence of the phase shifts on the atomic momentum k is shown in Fig. 4 for the five values of the cutoff radius R_c. The values of R_c are decreasing in steps of $\Delta R_c = 0.025$ from $R_c = 23.215$. The decrease of the cutoff radius causes the enlarging of the potential well (see Table II), the growth of the potential strength, and the increase of the phase shifts at a given k value.

In accordance with Levinson's theorem, in the low-energy limit the phase shifts tend to $n_s\pi$, where n_s is the number of bound states. For four larger values of R_c there are 58 bound states, whereas for $R_c = 23.115$
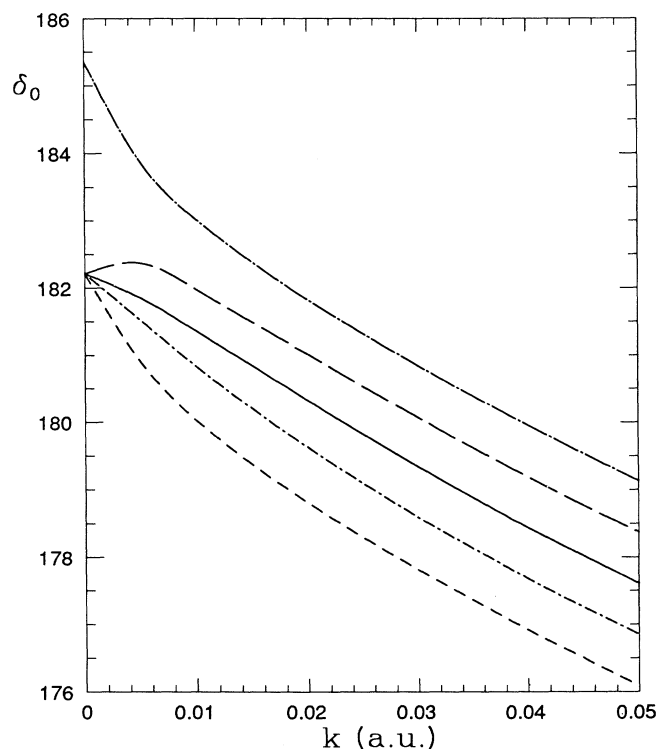

FIG. 4. The s-wave phase shifts $\delta_0(k)$ for the Cs-Cs $^3\Sigma_u$ scattering calculated with different values of the potential cutoff radius: short-dashed curve, $R_c = 23.215$ a.u.; dot-short-dashed curve, $R_c = 23.190$ a.u.; solid curve, $R_c = 23.165$ a.u.; long-dashed curve, $R_c = 23.140$ a.u.; dot-long-dashed curve, $R_c = 23.115$ a.u.

TABLE II. The Cs$_2$ $^3\Sigma_u$ potential and the scattering length.

R_c (a.u.)	R_0 (a.u.)	$R_{\min}$ (a.u.)	$U_{\min}$ (10^{-3} a.u.)	a^a (a.u.)	a^b (a.u.)
23.215	9.930	11.93	-1.273	376	352.5
23.190	9.906	11.91	-1.286	140	144.2
23.165	9.882	11.88	-1.300	65	68.0
23.140	9.856	11.86	-1.313	-69	-67.7
23.115	9.833	11.83	-1.327	467	485.3

^{a}Obtained by extrapolation of the s-wave phase shift towards zero k values.
^{b}Calculated using semiclassical formula (18).

the phase shift at $k \to 0$ jumps to 59π. The scattering lengths are found by the extrapolation of the phase shifts from the lowest calculated value at $k = 0.005$ a.u. to $n_s\pi$ at $k = 0$. The values of

$$a = - \lim_{k \to 0} \frac{d\delta_0}{dk}$$

are given in the fifth column of Table II. It should be noted that the numerical calculation of this limit produces large uncertainties, especially for large a values, when the phase shift is steep near $k = 0$. It follows from the general consideration of Sec. II that positive values of the scattering length well prevail over negative ones. This fact correlates with mostly decreasing behavior of the phase shifts in Fig. 4.

It is relevant now to compare the values of the scattering length, obtained from the solution of the Schrödinger equation to those calculated using our formulas (18) and (19). In the case of the Cs-Cs interaction $n = 6$, $\alpha = C_6$, and the mean scattering length $\bar{a}$ is

$$\bar{a} = \cos\left(\frac{\pi}{4}\right) \left(\frac{\sqrt{2MC_6}}{4}\right)^{1/2} \frac{\Gamma(\frac{3}{4})}{\Gamma(\frac{5}{4})} \simeq 95.5 \text{ a.u.}$$

This is the magnitude of the characteristic scattering length for the collision of ground-state cesium atoms. Using the potential (25) we calculated the semiclassical phase Φ (19) numerically with the help of (17), in order to estimate the contribution of the infinite upper limit precisely. The scattering lengths, obtained from (18), are presented in the last column of Table II. They are remarkably close to the values in the previous column. Furthermore, the semiclassical formula gives much more accurate results than the extrapolation of the phase shift. The number of bound states can also be obtained from Φ (19). It follows from condition (20) that

$$n_s = \left[\frac{\Phi}{\pi} - \frac{n-1}{2(n-2)}\right] + 1 , \qquad (27)$$

where [ ] means the integer part of the expression.

We would like to stress that the mean scattering length $\bar{a}$ governs the linear drop of the phase shifts at $k > \bar{a}^{-1} \simeq 0.01$: $\delta_0(k) \sim \Phi - \bar{a}k$. Indeed, at $k > 0.01$ all phase-shift curves in Fig. 4 are "parallel" with a slope of about $-\bar{a}$. On the contrary, at $k < \bar{a}^{-1}$ the behavior of the phase shifts is different, and the value of the scattering length strongly depends on the exact shape of the po-

tential well. The point is that the zero-energy scattering displays a resonant character, since often there is a bound or a virtual (resonant) energy level close to the threshold. We can describe it by the formula for the phase shift near resonance:

$$\delta_0(k) \simeq -\bar{a}k - \arctan\frac{k}{\kappa} + n_s\pi \quad (k < \bar{a}^{-1}) \tag{28}$$

and

$$a = \bar{a} + \frac{1}{\kappa} = \bar{a}\left[1 + \frac{1}{\bar{a}\kappa}\right]. \tag{29}$$

Here κ gives the position of the upper bound level $(\kappa > 0, \quad E_0 = -\frac{\kappa^2}{2M})$, or corresponds to the virtual level $(\kappa < 0)$, and the formula (29) has the structure of (3) or (18). When the number of levels in the well is large, the position of the upper level is extremely sensitive to small changes of the potential. However, if we consider the scattering process far from the resonance at $k \gg \kappa$, the behavior of the phase shift is steady, i.e., not sensitive to small variations of the potential, its slope being determined by the average value $\bar{a}$ of the scattering length.

It is interesting to apply formulas (18) and (19) to the case of H-H scattering. The H_2 $^3\Sigma_u$ potential is shallow, and rigorously speaking it hardly can be treated semiclassically. For the potential we use the same approximation (25) (see the parameters in Table I) with $f_c(R) \equiv 1$, because all the C_i are relatively small. The $1/R^n$ divergence appears only at $R < 4$, which is well to the left of the classical turning point $R_0 = 7.008$. The numerical solution of the Schrödinger equation for positive energy and extrapolation of the phase shift yields the value of $a = 1.42$. Using the semiclassical approach we have obtained $\bar{a} = 4.92$, $\Phi = 1.03$, and $a = 1.25$. Therefore, we see that the semiclassical approximation produces quite reasonable results far beyond the domain of its strict validity. We would like to stress that this agreement is not coincidental. The scattering length a is much smaller than $\bar{a}$, and it was essentially determined by the phase Φ. Let us also note that both values of a are close to the value of Friend and Etters [7], $a = 1.36a_B$, which was obtained using a slightly different approximation for the potential.

IV. CONCLUSIONS

Using the matching of the WKB approximation and the exact solution, we have obtained a formula for the scattering length of the potential with $-\alpha/R^n$ asymptotic behavior. It expresses the scattering length a in terms of the mean value $\bar{a}$, determined by the asymptotic behavior of the potential, and the phase-dependent factor, which strongly depends upon the actual shape of the potential well. Near the threshold scattering has a resonant character, and is very sensitive to the slightest changes of the potential. However, beyond the near-threshold region of $k < \bar{a}^{-1}$, the phase shifts display linear behavior, governed by the mean scattering length $\bar{a}$. It suggests the possibility of obtaining a more general formula for $\delta_0(k)$. That formula should connect the

TABLE III. Cs-Cs scattering phase shifts and cross sections.

k (a.u.)	Energy (μK)	$\delta_0{}^a$	σ^a (10^4 a.u.)	$\delta_0{}^b$	σ^b (10^4 a.u.)
0.003	12	182.02	5.1	182.37	3.4
0.005	33	181.85	6.3	182.37	1.2
0.007	64	181.67	6.8	182.25	0.0
0.010	130	181.36	7.1	181.98	0.7
0.012	187	181.15	6.7	181.78	1.5
0.014	255	180.95	5.8	181.59	2.2
0.016	333	180.73	4.9	181.38	2.7

[a] Obtained using the potential with $R_c = 23.165$ a.u. ($a = 65$ a.u.).
[b] Obtained using the potential with $R_c = 23.140$ a.u. ($a = -69$ a.u.).

range of $k < \bar{a}^{-1}$, in which the phase shift is determined by the scattering length (18), or, more accurately, by the resonance equation (28), to the region of larger k values. A comparison with the results of the numerical solution of the Schrödinger equation shows that the semiclassical approximation yields correct results even when the potential is shallow, and the wave function within the potential well does not oscillate at all.

Using a simple analytical approximation for the Cs_2 $^3\Sigma_u$ potential we have investigated the typical behavior of the s-wave phase shifts at small energies. The uncertainties of the potential does not allow to calculate the exact magnitude of the scattering length. However, it is possible to make some estimates. Recently the cross section has been measured for the elastic scattering of spin-aligned Cs atoms [9]. The experiment shows that the cross section is $1.5(4) \times 10^{-12}$ cm^2, and is approximately constant from 30 to 250 μK. This value is consistent with the scattering length of $a \simeq \pm 70$. We omit here the evaluation of the Bose-statistics effects, which depend upon a particular total spin component. In Table III we present the s-wave scattering cross sections for the potential (25) with $R_c = 23.165$ and 23.140. The scattering lengths for the two cases are 68.0 and -67.7, respectively (see Table II). For the positive a value the cross section is very flat, whereas for the negative one the cross section has a deep trough. Therefore, the comparison of the calculation with the experimental data favors a positive Cs-Cs scattering length.

Our results show that in a cooled atomic-gas sample the interaction between atoms is with a "probability" of three to one repulsive, rather than attractive. This fact is important in the search for the Bose-gas instability. This possibility is considered in [11], provided the low-energy interaction of atoms is attractive.

[1] C. Monroe, W. Swann, H. Robinson, and C. Wieman, Phys. Rev. Lett. **65**, 1571 (1990).

[2] J. M. Doyle, J. C. Sandberg, I. A. Yu, C. L. Cesar, D. Kleppner, and T. J. Greytak, Phys. Rev. Lett. **67**, 603 (1991).

[3] L. D. Landau and E. M. Lifshitz, *Quantum Mechanics: Non-Relativistic Theory* (Oxford, Pergamon, 1965).

[4] W. Kolos and L. Wolniewicz, J. Chem. Phys. **43**, 2429 (1965); Chem. Phys. Lett. **24**, 457 (1974).

[5] M. Krauss and W. J. Stevens, J. Chem. Phys. **93**, 4236 (1990).

[6] W. Weickenmeier, U. Diemer, M. Wahl, M. Raab, W. Demtröder, and W. Müller, J. Chem. Phys. **82**, 5354 (1985).

[7] D. G. Friend and R. D. Etters, J. Low Temp. Phys. **39**, 409 (1980).

[8] A. A. Radtsig and B. M. Smirnov, *Parameters of Atoms and Atomic Ions Handbook* (Energoatomizdat, Moscow, 1986).

[9] C. R. Monroe, E. A. Cornell, C. A. Sackett, C. J. Myatt, and C. E. Wieman, Phys. Rev. Lett. **70**, 414 (1993).

[10] M. Ya. Amusia and L. V. Chernysheva, *Automated System for Atomic Structure Investigation* (Nauka, Moscow, 1983).

[11] V. V. Flambaum and E. A. Kuznetsov, in *Proceedings of NATO Advance Research Workshop on Singularities in Fluids, Plasmas and Optics, Heraklion, Greece, 1992* (in press).