Probabilities for low-energy small-angle scattering in collisions of neutral particles

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General and analytical expressions for probabilities for center-of-mass scattering into small angles ($0° \leq \vartheta \lesssim 3°$) in elastic neutral-neutral collisions with low impact energy ($0.05\ \mathrm{eV} \lesssim E \lesssim 0.5\ \mathrm{eV}$) are derived. Several theories of the differential scattering into the small angles are analyzed in order to establish the most reliable differential cross section for the collisions. The "best" cross section is then used to derive the corresponding (analytical) scattering probabilities. The approach is used to calculate the *absolute* values of the small-angle, low-energy differential cross sections and the scattering probabilities for the Li-Hg, Na-Hg, and K-Hg interactions.

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I. INTRODUCTION

In principle, the momentum transfer in binary collisions of neutral particles should be studied using the general formalism of quantum-mechanical scattering theory. The formalism is well-developed [1–4] but requires formulation and solution of complex and computationally demanding models of collisional dynamics. This, and the fact that accurate potentials of most of the neutral-neutral collisions common in applications are either unknown or uncertain, causes that rigorous quantum-mechanical descriptions of the particles dynamics are available only for a small number of neutral-neutral collisions. The situation is even worse in the case of low-energy collisions (that is, the collisions with impact energy of a fraction of an electronvolt) even though such collisions are common in thermal nonequilibria in numerous applications of interest to modern technology. The last decades of research on the subject have shown that the nonequilibria can be successfully studied using high-power computers and advanced computational methods if the dynamics of the individual collisions contributing to the nonequilibria can be described with a satisfactory accuracy and with a reasonable computational efficiency. Therefore an accurate, general and analytical theory of the low-energy collisions of neutral particles would be of significant benefit for studies of thermal nonequilibria in a variety of applications. Derivation of such an "ideal" theory is practically impossible but approximate theories of this kind can be developed. Such theories are still very useful in studies of the thermal nonequilibria because: (1) measured scattering cross sections for most collision systems are not available; (2) preliminary analyses that usually precede formulation of state-of-the-art, large-scale models of the nonequilibria require easy-to-access information about the relative role of various collisions present in the nonequilibria; and (3) the theories are able to predict *absolute* values of the differential cross sections and corresponding scattering probabilities with accuracy acceptable in most applications.

We study below several analytical and semianalytical scattering theories of low-energy, small-angle binary elastic collisions of neutrals, and the "best" of the theories is used to formulate the present approach that yields general and analytical expressions for the differential cross sections and scattering probabilities for the collisions. The expressions are used to calculate the differential cross sections and scattering probabilities for the low-energy, small-angle elastic scattering in the Li-Hg, Na-Hg, and K-Hg systems where all atoms are in their ground states [Li($2s\ ^2S_{1/2}$), Na($3s\ ^2S_{1/2}$), K($4s\ ^2S_{1/2}$), and Hg($6s^2\ ^1S_0$)]. These interactions are chosen here because they are among the most carefully studied during the last several decades and, as a result, the recently proposed potentials for the interactions seem to be quite accurate. (However, neither absolute nor relative differential cross sections for the low-energy scattering of the systems into the angles between 0° and 3° are available in literature of the subject, a situation typical for most of the neutral-neutral interactions common in applications.) In addition, the energies of the first excited levels of the Li, Na, K, and Hg atoms (the levels $2p\ ^2P^0_{1/2}$, $3p\ ^2P^0_{1/2}$, $4p\ ^2P^0_{1/2}$, and $6p\ ^3P^0_0$, respectively) are large enough (1.848, 2.102, 1.610, and 4.667 eV, respectively) to maintain a high population of these ground-state atoms in systems under thermal conditions (see below).

II. THE LOW ENERGY COLLISIONS

The temperatures of neutral particles in most gases, vapors, and partially ionized plasmas of interest in modern applications are between a few hundred Kelvins and a few thousand Kelvins. Thus most of neutral particles in the applications have kinetic energies between 0.05 and 0.5 eV. Such energies are called below "low energies" or "thermal energies," and the applications with most of the neutral particles having such energies are considered as being under "thermal conditions." (Most of the existing work on the neutral-neutral elastic collisions has been done on large- and medium-energy scattering into small and large angles, while much less research is available on the low-energy scattering of neutral particles into the small angles.)

The defined above "low-energy" interactions can usually be considered "slow" collisions, that is, the collisions where the ratio κ of the particles relative speed w to the Massey-

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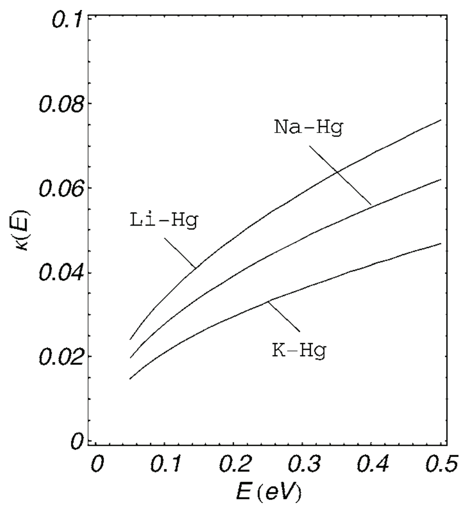

FIG. 1. The energy dependence of ratio (2) for the Li-Hg, Na-Hg, and K-Hg interactions.

Mohr characteristic speed w_{mm} [5,6] is much smaller than one,

$$\kappa(E) \ll 1, \tag{1}$$

where

$$\kappa(E) = \frac{w}{w_{mm}} = \frac{\hbar}{r_0 D}\left(\frac{2E}{\mu}\right)^{1/2}, \tag{2}$$

where $\hbar = h/2\pi$ (h is Planck's constant), μ is the collision reduced mass, r_0 is the distance between particles at which the interaction potential has its minimum, D is the potential well-depth, and

$$E = \mu w^2/2 \tag{3}$$

is the impact energy of the collision.

The ratios (2) for the Li-Hg, Na-Hg, and K-Hg interactions are shown in Fig. 1. The ratios were calculated assuming the following values of the parameters r_0 (in bohrs) and D (in eV) of the actual interaction potentials: r_0=5.52 (Li-Hg), 6.66 (Na-Hg), 7.37 (K-Hg), and D=0.112 (Li-Hg), 0.065 (Na-Hg), 0.062 (K-Hg) (see Ref. [7] and discussion below).

III. THE INTERACTION POTENTIALS

Since most of the low-energy, small-angle neutral-neutral collisions in applications under thermal conditions have the ratio (2) much smaller than one, the collisions are driven mainly by the attractive forces between the particles [4–6,8]. Therefore one can assume in the physical model of the collisions that their interaction potential $U(r)$ is

$$U(r) = U_{rep}(r) + U_{att}(r) = \frac{C_n}{r^n} - \frac{C_s}{r^s} \simeq -\frac{C_s}{r^s}, \tag{4}$$

where r is the distance between the particles, $U_{rep}(r)$ and $U_{att}(r)$ are the repulsive and attractive parts of the potential, respectively, and C_n, C_s, n, and s are some positive constants.

In typical neutral-neutral collisions, the values of s are equal or close to six. The potential exponent s can differ (but not much) from six since the actual long-range potential can contain higher-order terms ($-C_8/r^8$, $-C_{10}/r^{10},\ldots$) making s in the single-term function (4) being slightly different from six. Therefore the expressions for the differential cross sections derived in this work are valid when s is close to six, say $5.5 \lesssim s \lesssim 6.5$.

The assumption that the discussed collisions are dominated by the attractive potential $-C_s/r^s$ is usually well-justified. The assumption is also very convenient in theoretical studies of the collisions since it allows one to make a number of mathematical simplifications which permit derivation of analytical expressions for the differential cross sections and scattering probabilities of interest here.

The potential energy of the Li-Hg interaction was studied by molecular beam scattering experiments [9–12], by laser-assisted spectroscopy [13–15], and by all-electron *ab initio* calculations [16].

The potential energy of the Na-Hg interaction was studied by molecular beam experiments [17,18], by pseudopotential calculations [19], and by relativistic all-electron *ab initio* calculations [20,21].

The potential energy of the K-Hg interaction was studied by molecular beam experiments [22–24] and by pseudopotential calculations [19].

The research on the Li-Hg, Na-Hg, and K-Hg interactions was critically reviewed recently by Thiel *et al.* [7]. Their analysis, supplemented by their own pseudopotential calculations of the potential energies and various multiproperty fits, recommended the potential curves that seem to be quite realistic representations of the scattering forces in the interactions.

General methods of calculating the potential constants C_s for different types of collision systems are available in literature of the subject (see reviews [25,26] and references therein). In this paper, we calculated the constants for the Li-Hg, Na-Hg, and K-Hg collisions using the results of the review of Thiel *et al.* [7] where Fig. 3 (for the Li-Hg collision), Fig. 7 (for the Na-Hg collision), and Fig. 12 (for the K-Hg collision) show the energy-dependences of the products $\sigma_{tot}(E)E^{1/5}$ recommended for the collisions [$\sigma_{tot}(E)$ are the total (integral) elastic cross sections for the discussed interactions]. We chose from the figures the mean values of the oscillating (with energy) products $\sigma_{tot}(E)E^{1/5}$ (600 bohr^2 hartree$^{1/5}$ for the Li-Hg collision, 700 bohr^2 hartree$^{1/5}$ for the Na-Hg collision, and 1000 bohr^2 hartree$^{1/5}$ for the K-Hg collision) at energies E_0 corresponding to these mean values while being close to the middle value (E=0.25 eV) of the considered range of the "low" impact energy (E_0=0.272 eV for the Li-Hg collision, E_0=0.227 eV for the Na-Hg collision, and E_0=0.247 eV for the K-Hg collision). The resulting values of the total cross sections are: $\sigma_{tot}(E_0)=4.220\times10^{-18}$ m^2 (Li-Hg), $\sigma_{tot}(E_0)$ $=5.106\times10^{-18}$ m^2 (Na-Hg), and $\sigma_{tot}(E_0)=7.169\times10^{-18}$ m^2 (K-Hg). These values were used to calculate the potential constants C_s needed in relationship (4). This is done by assuming that s=6 and that $\sigma_{tot}(E_0)=\sigma_{mm}(E_0)$, where $\sigma_{mm}(E_0)$ is the Massey-Mohr's total (integral) elastic cross section

[5,6] which is known to predict quite realistic values for collisions with relative speeds much smaller than the Massey-Mohr characteristic speed w_{mm}.

The Massey-Mohr total cross section for elastic binary collision of neutrals at initial relative speed w in the field of potential $-C_s/r^s$ is

$$\sigma_{mm}(w) = f_{mm}(s)\left(\frac{C_s}{\hbar w}\right)^{2/(s-1)}, \tag{5}$$

where

$$f_{mm}(s) = \pi\frac{2s-3}{s-2}[2p(s)]^{2/(s-1)}, \tag{6}$$

$$p(s) = \frac{\pi^{1/2}}{2}\frac{\Gamma[(s-1)/2]}{\Gamma[s/2]}, \tag{7}$$

and $\Gamma[y]$ is gamma function of argument y.

The relationship (6) differs from the one proposed originally by Massey and Mohr [5]; the values of $f_{mm}(s)$ in the relationship (6) are the more accurate ("corrected") values proposed by Bernstein and Kramer [6].

The relationship (5) and the assumption that $\sigma_{tot}(E_0) = \sigma_{mm}(E_0)$ give

$$C_s = \left[\frac{\sigma_{\text{tot}}(w_0)}{f_{mm}}\right]^{(s-1)/2}\hbar w_0, \tag{8}$$

where $w_0 = (2E_0/\mu)^{1/2}$. For $s=6$, the values of the potential constants C_6 for the Li-Hg, Na-Hg, and K-Hg interactions are 6.868×10^{-77} J m^6, 5.762×10^{-77} J m^6, and 1.115×10^{-76} J m^6, respectively.

IV. THE DIFFERENTIAL CROSS SECTIONS

The differential cross section for center-of-mass scattering of two neutral particles of a low impact energy E into a small angle ϑ can be given as [1–4]

$$I(E,\vartheta) \simeq |f(E,\vartheta|^2, \tag{9}$$

where $f(E,\vartheta)$ is the collision scattering amplitude obtained from solution of the time-independent wave equation for the collision at a (positive) total energy E in the potential field of the fixed scattering center.

The transformation of the center-of-mass cross section $I(E,\vartheta)$ to the corresponding laboratory cross section $Q(E,\theta)$ is [4]

$$Q(E,\theta) = \frac{[(m_1 m_2)^2 + 2(m_1/m_2)\cos\vartheta + 1]^{3/2}}{1+(m_1/m_2)\cos\vartheta}I(E,\vartheta), \tag{10}$$

where ϑ and θ are the scattering angles in the center-of-mass frame and in the laboratory frame, respectively, and m_1 and m_2 are masses of the interacting particles.

We discuss below four analytical models (called models A, B, H, and M) of elastic scattering of neutrals particles into an angle ϑ between 0° and 3° at impact energies E between 0.05 and 0.5 eV. The models have been most commonly discussed in the literature of the subject [1–4].

A. The model A

This model was proposed by Anderson [27] who formulated the small-angle differential cross section for elastic interaction of neutral particles in the field of the potential (4) as a product of the classical differential cross section for the interaction and the so-called "quantum correction factor" representing the departure of the real cross section from the classical one. The correction factors were obtained using the usual partial wave expansion for the quantum-mechanical scattering amplitude, replacing the sum by an integral, and replacing the phase shifts in the sum by their Jeffreys-Born values. The resulting center-of-mass differential cross section for neutral-neutral scattering into small angles at low impact energy is [3,27]

$$I_A(E,\vartheta) = f_s(s,\gamma_s)I_c(E,\vartheta), \tag{11}$$

where $I_c(E,\vartheta)$ is the classical differential cross section for the scattering into small angles,

$$I_c(E,\vartheta) = [2(s-1)A_s]^{2/s}k^{-2/s}[s\vartheta^{(s+2)/s}\sin\vartheta]^{-1}, \tag{12}$$

$$A_s = p(s)C_s/\hbar w, \tag{13}$$

the wave number of the relative motion of the interacting particles is

$$k = \mu w/\hbar, \tag{14}$$

and the quantum correction factor $f_s(s,\gamma_s)$ is

$$f_s(s,\gamma_s) = s[2(s-1)]^{-2/s}R(s,\gamma_s), \tag{15}$$

with

$$R(s,\gamma_s) = [R_1(s,\gamma_s)]^2 + [R_2(s,\gamma_s)]^2, \tag{16}$$

$$R_1(s,\gamma_s) = 4\int_0^\infty \sin^2[\gamma_s^{(s^2-1)/2s}x^{1-s}]J_0[\gamma_s^{(s-1)/2s}x]x\,dx, \tag{17}$$

$$R_2(s,\gamma_s) = \int_0^\infty \sin[2\gamma_s^{(s^2-1)/2s}x^{1-s}]J_0[\gamma_s^{(s-1)/2s}x]x\,dx, \tag{18}$$

$$\gamma_s = \vartheta/\vartheta_s, \tag{19}$$

and

$$\vartheta_s = A_s^{1/(1-s)}/k, \tag{20}$$

where $J_0[y]$ is the Bessel function of argument y.

The correction factors $f_s(s,\gamma_s)$ are very close to one when $\gamma_s > 5$ and when the potential exponent s is between 5 and 7. The integrals (17) and (18) are strongly oscillatory and cannot be obtained in closed analytical forms. Calculating highly accurate values of the integrals is time-consuming and requires use of advanced numerical methods. Therefore we approximated (with accuracy better than 1%) the results of such calculations by the following relationships convenient for the quantitative studies of the collisions under consideration:

TABLE I. The coefficients a_i in the polynomial (21) for the potential exponents $s=5.5$, 6, and 6.5.

i	$s=5.5$	$s=6$	$s=6.5$
0	0.00058263	−0.00228972	−0.00430805
1	−0.02384629	0.10343309	0.18401837
2	1.05721252	0.28192746	−0.13500409
3	4.23218612	5.59555087	6.21005104
4	−7.11532543	−7.99856858	−8.16220084
5	4.42315478	4.63641475	4.47507660
6	−1.42906960	−1.41993098	−1.29826548
7	0.25714871	0.24332495	0.20996758
8	−0.02456235	−0.02216940	−0.01795384
9	0.00097514	0.00084016	0.00063434

$$f_s(s,\gamma_s) = \sum_{i=0}^{9} a_i \gamma_s^i \quad \text{when } 0 \leqslant \gamma_s \leqslant 5, \tag{21}$$

$$f_s(s,\gamma_s) = 1 \quad \text{when } \gamma_s > 5. \tag{22}$$

The coefficients a_i for the potential exponents $s=5$, $s=5.5$, $s=6$, $s=6.5$, and $s=7$ are given in Tables I and II. The quantum correction factors for $s=5$, $s=6$, and $s=7$ are plotted in Fig. 2.

The dependence of the angle ϑ_s on the impact energy in the Li-Hg, Na-Hg, and K-Hg collisions is shown in Fig. 3.

One should notice that even small deviations of the functions $f_s(s,\gamma_s)$ and $I_c(E,\vartheta)$ from their accurate values can cause large errors in the values of the cross section $I_A(E,\vartheta)$ when ϑ approaches zero [the cross section $I_c(E,\vartheta)$ approaches infinity then]. However, as indicated by all quantum-mechanical theories of scattering, the derivative $\partial I_A(E,\vartheta)/\partial\vartheta$ is then close to zero in the entire range of the impact energy considered in this paper. Therefore we assume in what follows that when $0 \leqslant \vartheta \leqslant 0.2\vartheta_s$, the cross section (11) is

$$I_A(E,\vartheta \leqslant 0.2\vartheta_s) = f_s(s,\gamma_s=0.2) I_c(E,\vartheta=0.2\vartheta_s), \tag{23}$$

where

TABLE II. The coefficients a_i in the polynomial (21) for the potential exponents $s=5$ and 7.

i	$s=5$	$s=7$
0	0.00395791	−0.00551545
1	−0.19371599	0.22596983
2	2.24963443	−0.28600913
3	1.91332034	6.30869363
4	−5.25124067	−7.86406046
5	3.66878364	4.09087487
6	−1.26637854	−1.11509787
7	0.23945546	0.16692826
8	−0.02384686	−0.01293307
9	0.00098230	0.00040126

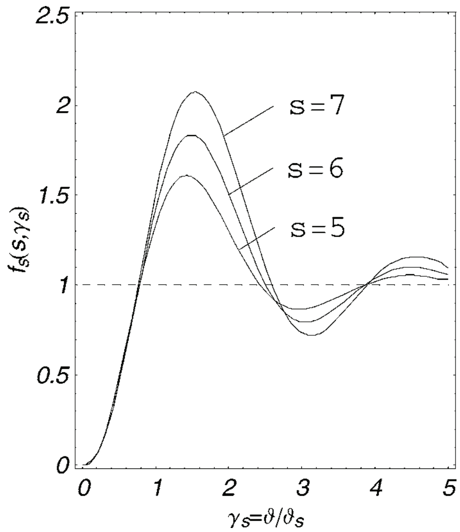

FIG. 2. The quantum correction factors $f_s(s,\gamma_s)$ [Eq. (21)] for potential exponents $s=5$, 6, and 7.

$$f_s(s,\gamma_s=0.2) \simeq f_s(s=6,\gamma_s=0.2) = 0.062, \tag{24}$$

because the factor $f_s(s,\gamma_s=0.2)$ is a very weak function of the potential exponent s when $5 \leqslant s \leqslant 7$.

B. The model B

This model was proposed by Beijerinck *et al.* [28]. The model was based on least-squares fits of the real and imaginary parts of quantum-mechanical scattering amplitudes with a variety of model functions based on existing classical and quantum-mechanical results for small-angle scattering. The authors concluded that the center-of-mass differential cross section for low-energy scattering of neutral particles into small angles can be given as

$$I_B(E,\vartheta) = q_0(E)\beta_5\beta(E,\vartheta)(\vartheta/\vartheta_0)^{-2(s+1)/s}, \tag{25}$$

where

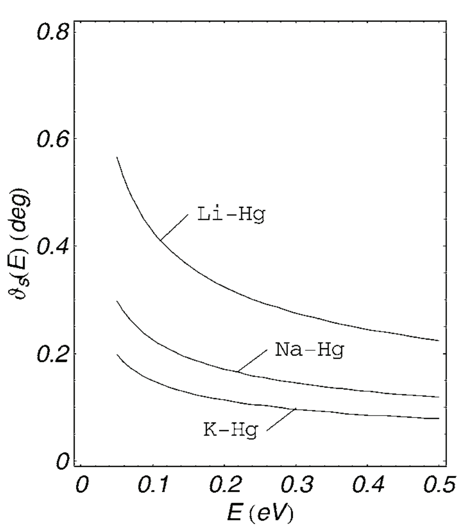

FIG. 3. The angle ϑ_s [Eq. (20)] for the low-energy Li-Hg, Na-Hg, and K-Hg collisions when $s=6$.

$$q_0(E) = \{(E/2)^{s-3}(\mu/\hbar^2)^{s+1}[p(s)C_s]^4\}^{1/(s-1)} \times\{\Gamma[(s-3)/(s-1)]\}^2, \quad (26)$$

$$\beta_1 = \frac{1}{2}\Gamma[(s-3)/(s-1)][p(s)]^{2/(s-1)}, \quad (27)$$

$$\beta_2 = \beta_1 \cos[\pi/(s-1)], \quad (28)$$

$$\beta_3 = 1 + \tan^2[\pi/(s-1)], \quad (29)$$

$$\beta_5 = \frac{(s-1)^{2/s}}{s}\frac{[p(s)]^{2/s}}{\beta_3\beta_2^{(s-1)/s}}, \quad (30)$$

$$\beta(E,\vartheta) = 1 + \exp(-2\beta_{15}\delta) + 2\exp(-\beta_{15}\delta) \times\cos(\beta_{16}\delta + \pi/s + \pi/2), \quad (31)$$

$$\delta = \beta_{14}(\vartheta/\vartheta_0)^{(s-1)/s}, \quad (32)$$

$$\beta_{14} = (s-1)^{1/s}\beta_2[p(s)]^{1/s}, \quad (33)$$

$$\beta_{15} = s(s-1)^{-1}\sin(\pi/s), \quad (34)$$

$$\beta_{16} = s(s-1)^{-1}[\cos(\pi/s)+1], \quad (35)$$

$$\vartheta_0 = \lambda_r^{-1}\{\mathrm{Im}[F(0,s)]\}^{-1/2}, \quad (36)$$

$$\lambda_r(E) = (2E)^{(s-2)/(2s-2)}[p(s)C_s(\mu^{1/2}/\hbar)^s]^{1/(s-1)}, \quad (37)$$

and

$$\mathrm{Im}[F(0,s)] = -i\int_0^\infty x[\exp(2ix^{1-s})-1]J_0(0)dx, \quad (38)$$

where $i=\sqrt{-1}$.

The integral (38) can be obtained in closed form for the following integral values of the potential exponent s:

$$\mathrm{Im}[F(0,s=4)] = -\frac{\Gamma[-2/3]}{3\times 2^{1/3}} = 1.06314, \quad (39)$$

$$\mathrm{Im}[F(0,s=5)] = \frac{\pi^{1/2}}{2} = 0.88620, \quad (40)$$

$$\mathrm{Im}[F(0,s=6)] = \frac{(1+5^{1/2})\Gamma[3/5]}{2^{13/5}} = 0.79486, \quad (41)$$

$$\mathrm{Im}[F(0,s=7)] = \frac{3^{1/2}\Gamma[2/3]}{2^{5/3}} = 0.73870, \quad (42)$$

$$\mathrm{Im}[F(0,s=8)] = \frac{3^{1/2}\Gamma[5/7]\sin(5\pi/14)}{2^{5/7}} = 0.70071. \quad (43)$$

Thus, when $5\leqslant s\leqslant 7$, the integral (38) can be approximated (with accuracy better than 1%) by the following quadratic function:

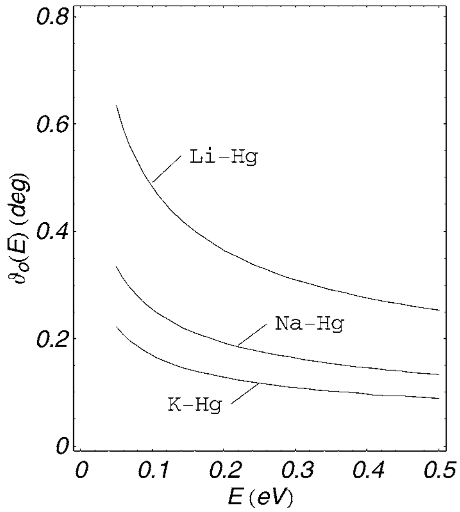

FIG. 4. The angle ϑ_0 [Eq. (36)] for the low-energy Li-Hg, Na-Hg, and K-Hg collisions when $s=6$.

$$\mathrm{Im}[F(0,s)] \simeq 1.8706 - 0.2848s + 0.0176s^2. \quad (44)$$

The relationships (25)–(38) resulted from using the work of Gordon [29] in the original approach of Beijerinck *et al.* [28]. The relationships were recommended by Beijerinck *et al.* as a general and reliable tool to study small-angle scattering of neutral particles. In addition, fitting of these and other similar expressions for various small-angle scattering cross sections for neutral particles led Beijerinck *et al.* to the following semiempirical center-of-mass differential cross section for low-energy, small-angle elastic scattering of neutral particles:

$$I_B(E,\vartheta) = q_0(E)\times\{1 - c_1\sin[c_2(\vartheta/\vartheta_0)^2] + c_3(\vartheta/\vartheta_0)^2\}^{-(s+1)/s}, \quad (45)$$

where $c_1=3.75$, $c_2=0.556$, $c_3=2.94$, and $q_0(E)$ is given in expression (26).

The dependence of the angle ϑ_0 [Eq. (36)] on the impact energy in the Li-Hg, Na-Hg, and K-Hg collisions is shown in Fig. 4.

C. The model H

This model was proposed by Helbing and Pauly [4,8,30]. The authors used in the model semiclassical approximation to the usual partial wave expansion of scattering amplitude, the random-phase approximation for evaluation of quantal phase shifts, and the inverse power interaction potential. Applicaton of their approach to low-energy, small-angle elastic scattering of neutral particles in the center-of-mass frame led to the following differential cross section for the scattering:

$$I_H(E,\vartheta) = 2^{(s+1)/(s-1)}\hbar^{-2}g_1\mu E\left[\frac{p(s)C_s\mu^{1/2}}{\hbar E^{1/2}}\right]^{4/(s-1)} \times\exp\left\{2^{s/(s-1)}g_2\mu E\left[\frac{p(s)C_s\mu^{1/2}}{\hbar E^{1/2}}\right]^{2/(s-1)}\frac{\vartheta^2}{\hbar^2}\right\}, \quad (46)$$

where $g_1=0.4275$ and $g_2=0.6091$.

D. The model M

This model was developed by Mason and co-workers [31–33] who used semiclassical approximation for the scattered amplitude, the random-phase approximation to calculate quantal phase shifts, and the inverse power interaction potential. Their center-of-mass differential cross section for the small-angle neutral-neutral scattering at low energy is

$$I_M(E,\vartheta)=\left[\frac{kS(0)}{4\pi}\right]^2\left[1+\tan^2\left(\frac{\pi}{s-1}\right)\right]\times\exp\left[-\frac{d(s)k^2S(0)\vartheta^2}{8\pi}\right], \quad (47)$$

where

$$S(0)=F(s)\left(\frac{C_s}{\hbar w}\right)^{2/(s-1)}, \quad (48)$$

$$d(s)=\left[\Gamma\left(\frac{2}{s+1}\right)\right]^2\left[2\pi\Gamma\left(\frac{4}{s-1}\right)\right]^{-1}\tan\left(\frac{2\pi}{s-1}\right), \quad (49)$$

$$F(s)=\pi^2\left[\frac{2K(s)}{s-1}\right]^{2/(s-1)}\left[\Gamma\left(\frac{2}{s-1}\right)\sin\left(\frac{\pi}{s-1}\right)\right]^{-1}, \quad (50)$$

$$K(s)=\pi^{1/2}\frac{\Gamma[(s+1)/2]}{\Gamma[s/2]}. \quad (51)$$

The relationship (47) cannot be used in the case of collisions where the potential exponent s is smaller than or equal to five [31].

V. COMPARISON OF THE MODELS A, B, H, AND M

The small-angle center-of-mass differential cross sections $I_A(E,\vartheta)$, $I_B(E,\vartheta)$, $I_H(E,\vartheta)$, and $I_M(E,\vartheta)$ (of the scattering models A, B, H, and M, respectively) for the Li-Hg, Na-Hg, and K-Hg interactions at a low energy (E=0.25 eV) are shown in Figs. 5–7. One can see in the figures that the models A and B give very similar values of the small-angle differential cross sections for all considered interactions at this impact energy. The cross sections are also very close at other energies within the 0.05 eV$\lesssim E \lesssim$0.5 eV range. This seems to be a strong argument for considering the cross sections of models A and B as the "best" analytical tools for studying the low-energy, small-angle scatterings in the Li-Hg, Na-Hg, and K-Hg collisions and for many other collision systems. Subsequently, either the cross section $I_A(E,\vartheta)$ or the cross section $I_B(E,\vartheta)$ can be used to study the collisions; we choose for this purpose the cross section $I_B(E,\vartheta)$ given in expression (45).

Figures 5–7 also show that the models H and M are inadequate representations of the dynamics of the discussed collisions. Even at the scattering angles very close to zero, the differential cross sections proposed by these two models should be treated as crude estimates.

In general, the accuracy of the cross section $I_B(E,\vartheta)$ increases with a decrease of the impact energy E because the energy decrease diminishes the role of the repulsive part of the actual interaction of the particles. The accuracy also depends on the accuracy of the long-range potentials (that is, on the accuracy of the constants C_s and s).

The cross section $I_B(E,\vartheta)$ can also be used to describe many atom-molecule and molecule-molecule small-angle elastic collisions in systems under thermal conditions. However, one has to consider in such cases the fact that the scatterings involving molecules may depend meaningfully on the molecular configuration, and that the way of averaging over the possible configurations may not be obvious (see Ref. [35] and references therein).

Taking s=6, the cross section (45) can be written as

$$I_B(E,\lambda)=q_0(E)\Omega(\lambda), \quad (52)$$

where

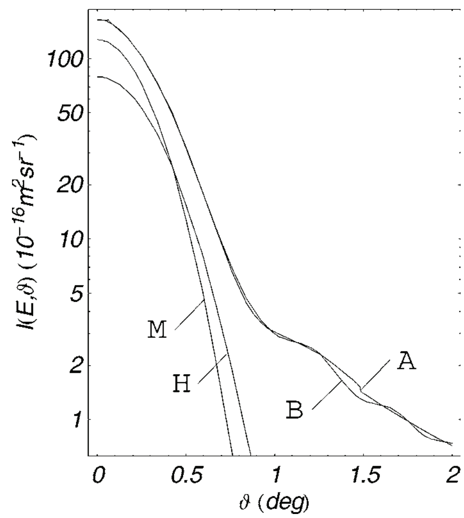

FIG. 5. Comparison of the center-of-mass differential cross sections discussed in the text for the Li-Hg collision when s=6 and E=0.25 eV. The cross sections $I_A(E,\vartheta)$, $I_B(E,\vartheta)$, $I_H(E,\vartheta)$, and $I_M(E,\vartheta)$, are marked, respectively, by the letters A, B, H, and M.

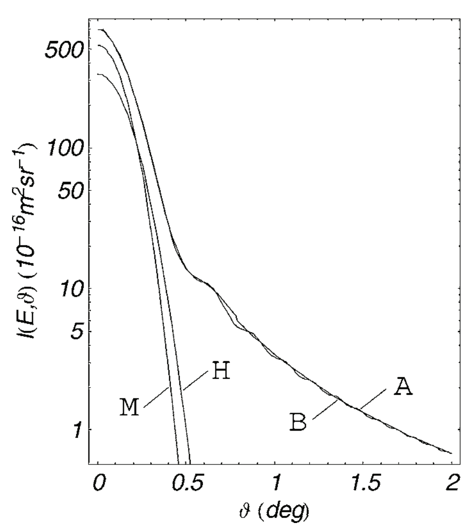

FIG. 6. Comparison of the center-of-mass differential cross sections discussed in the text for the Na-Hg collision when s=6 and E=0.25 eV. The meaning of the symbols is the same as in Fig. 5.

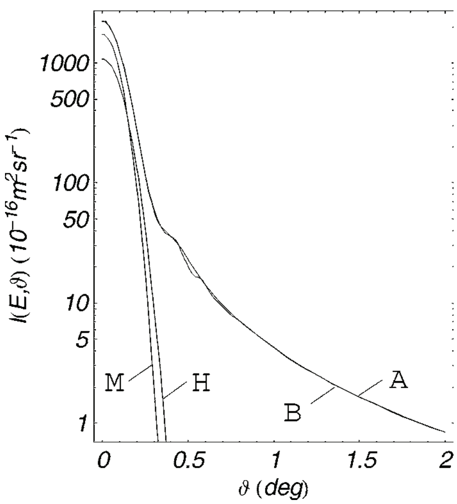

FIG. 7. Comparison of the center-of-mass differential cross sections discussed in the text for the K-Hg collision when $s=6$ and $E=0.25$ eV. The meaning of the symbols is the same as in Fig. 5.

$$q_0(E) = 0.9581\left(\frac{C_6^4 E^3 \mu^7}{\hbar^{14}}\right)^{1/5}, \tag{53}$$

$$\Omega(\lambda) = [1 + c_3\lambda^2 - c_1 \sin(c_2\lambda^2)]^{-7/6}, \tag{54}$$

$$\lambda = \vartheta/\vartheta_0, \tag{55}$$

and

$$\vartheta_0(E) = 0.9447\left(\frac{\hbar^6}{\mu^3 E^2 C_6}\right)^{1/5}. \tag{56}$$

The expression in the square brackets in relationship (54) can be approximated by the following "undulation-averaged" expression

$$1 + c_3\lambda^2 - c_1 \sin(c_2\lambda^2) \simeq 2.956\lambda^2, \tag{57}$$

when $\lambda^2 \gtrsim 1$ ($\vartheta_0 \lesssim \vartheta \lesssim 3°$) and when the collision constants have the following value: 5×10^{-79} J m$^6 \lesssim C_6 \lesssim 5\times10^{-77}$ J m^6, 4 amu$\lesssim \mu \lesssim$100 amu, and 0.05 eV$\lesssim E \lesssim$0.5 eV. Most of the neutral-neutral interactions of interest in technology have the collision constants within these intervals.

Use of the relationship (57) in the expression (52) leads to

$$I_B(E,\vartheta) \simeq 0.237(C_6/E)^{1/3}\vartheta^{-7/3} \tag{58}$$

when $\vartheta_0 \lesssim \vartheta \lesssim 3°$. [When $\vartheta \simeq 0$, the cross section is given by expression (53).]

One can see in relationship (53) that the differential cross section for the low-energy neutral-neutral scattering into angles very close to $\vartheta=0°$ has a distinctive (stronger than linear) dependence on the reduced mass μ but no dependence on μ is seen in the cross section (58) valid for the scattering angle greater than ϑ_0.

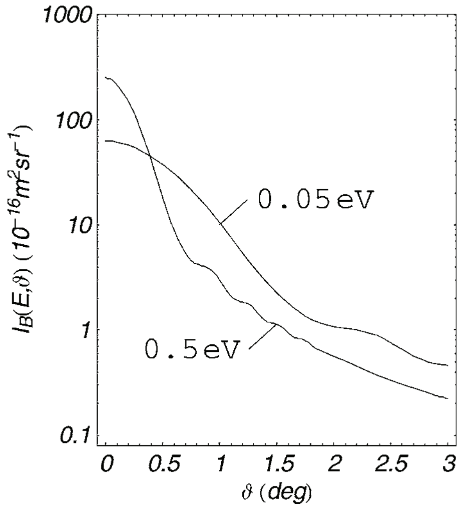

FIG. 8. The center-of-mass differential cross section $I_B(E,\vartheta)$ for the Li-Hg scattering into small angles ϑ at low impact energies when $s=6$.

The cross sections (53) and (58) both increase with increase of the potential constant C_6, but the dependences of the cross sections on the impact energy E differ significantly: the cross section (53) increases with the energy while the cross section (58) decreases with the energy.

It is also worthy to notice in relationship (58) the expected ϑ-dependence ($\sim\vartheta^{-7/3}$) of the cross section $I_B(E,\vartheta)$ for scattering in angles $\vartheta_0 \lesssim \vartheta \lesssim 3°$.

The center-of-mass classical differential cross section for elastic scattering of two rigid spheres is [3]

$$I_{crs}(E,\vartheta) = (d_0/2)^2, \tag{59}$$

and the corresponding classical total cross section is

$$\sigma_{crs}(E) = \pi d_0^2, \tag{60}$$

where d_0 (the so-called "collision diameter") is the sum of the radii of the spheres participating in the collision.

The center-of-mass quantum-mechanical differential cross section and the corresponding quantum-mechanical total cross section for elastic scattering of two rigid spheres are, respectively [3],

$$I_{qrs}(E,\vartheta) = d_0^2 \tag{61}$$

and

$$\sigma_{qrs}(E) = 4\pi d_0^2. \tag{62}$$

We calculated the collision diameters for the Li-Hg, Na-Hg, and K-Hg systems using the mean radii of the outer atomic shells [36]. The resulting classical rigid-sphere differential cross sections are 3.63×10^{-20} m^2 sr^{-1} (Li-Hg), 3.98×10^{-20} m^2 sr^{-1} (Na-Hg), and 5.14×10^{-20} m^2 sr^{-1} (K-Hg), and the quantal rigid-sphere differential cross sections are 1.45×10^{-19} m^2 sr^{-1} (Li-Hg), 1.59×10^{-19} m^2 sr^{-1} (Na-Hg), and 2.06×10^{-19} m^2 sr^{-1} (K-Hg). The classical rigid-sphere total cross sections are 4.56×10^{-19} m^2 (Li-Hg), 5.01×10^{-19} m^2 (Na-Hg), and 6.46×10^{-19} m^2 (K-Hg), and the quantal rigid-sphere total cross sections are 1.82×10^{-18} m^2

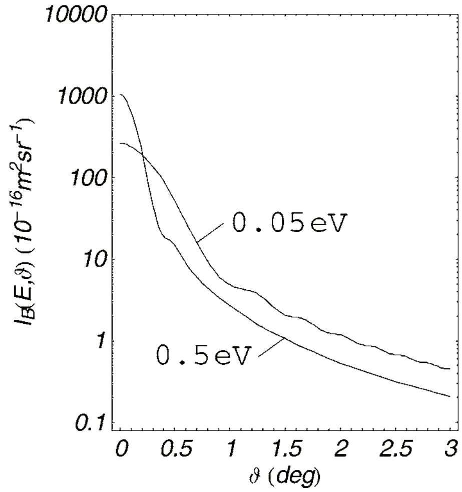

FIG. 9. The center-of-mass differential cross section $I_B(E,\vartheta)$ for the Na-Hg scattering into small angles ϑ at low impact energies when $s=6$.

(Li-Hg), 2×10^{-18} m^2 (Na-Hg), and 2.58×10^{-18} m^2 (K-Hg). Comparison of these values with the results given in Figs. 5–10 confirms the fact that the rigid-sphere model is an inadequate representation of low-energy, small-angle elastic scattering of neutral particles.

If the collision diameter for a collision under consideration is not available then one can estimate the diameter as follows. First, one can assume that the collision is driven by a generalized Lennard-Jones potential,

$$U(r)=\frac{sD}{n-s}\left[\left(\frac{r_0}{r}\right)^n-\frac{n}{s}\left(\frac{r_0}{r}\right)^s\right], \tag{63}$$

so that the collision diameter for interactions where $n\neq s$ can be given as [34]

$$d_0=\left(\frac{s}{n}\right)^{1/(n-s)}r_0. \tag{64}$$

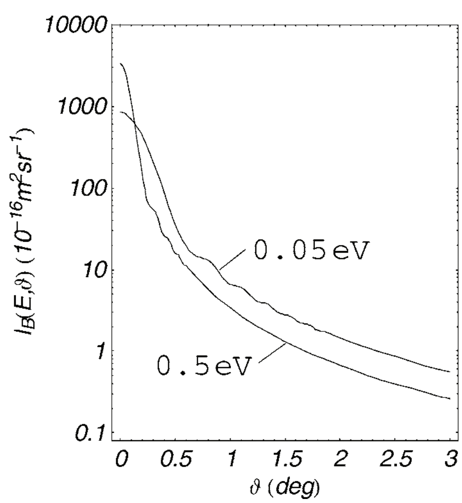

FIG. 10. The center-of-mass differential cross section $I_B(E,\vartheta)$ for the K-Hg scattering into small angles ϑ at low impact energies when $s=6$.

The typical exponents n of short-range potentials of neutral-neutral elastic collisions in vicinity or $r=d_0$ are between 5 and 12. For $s=6$ (s is always close to six), the values of diameter (64) are $0.855r_0$ (when $n=5$) and $0.903r_0$ (when $n=12$). Thus assuming that d_0 for the neutral-neutral elastic collisions is equal to $0.866r_0$ [the value of expression (64) for $n=8$] gives acceptable estimates of the collision diameters for most of the interactions of interest in applications. The value $d_0=0.866r_0$ is very close to the value $d_0=0.87r_0$ recommended for many neutral-neutral collisions in a general analysis of the transport effects of the collisions [34].

VI. THE ABSOLUTE DIFFERENTIAL CROSS SECTIONS FOR THE LI-HG, NA-HG, AND K-HG COLLISIONS

The absolute center-of-mass differential cross sections for the small-angle scattering in the Li-Hg, Na-Hg, and K-Hg interactions at energies of 0.05 and 0.5 eV were calculated using the relationship (45) and the potential parameters discussed above. The cross sections are shown in Figs. 8–10. The cross sections have strong peaks at very small angles, and the magnitudes of the peaks as well as the cross sections at larger angles depend on both the interaction potential and impact energy. Since the potential constants C_6 for the interactions were obtained from a rather rigorous analysis [7], the results shown in Figs. 8–10 should be a realistic representation of the small-angle scattering in the Li-Hg, Na-Hg, and K-Hg collisions at low energy. Unfortunately, no measured cross sections for the collisions are available to test the accuracy of the results.

VII. THE TOTAL CROSS SECTION

We assume in what follows that the total (integral) cross section $\sigma_{tot}(E)$ for low-energy elastic scattering of neutral particles under thermal conditions can be approximated by the "corrected" Massey-Mohr integral cross section [4–6]. The "corrected" cross section $\sigma_{MM}(E)$ is a sum of the "original" Massey-Mohr integral cross section $\sigma_{mm}(E)$, and a correction $\Delta\sigma(E)$ accounting for the glory contributions,

$$\sigma_{tot}(E)=\sigma_{MM}(E)=\sigma_{mm}(E)+\Delta\sigma(E), \tag{65}$$

with

$$\Delta\sigma(E)=-4\pi r_0^2\frac{\beta_0(E)}{|\gamma_0(E)|^{1/2}}\left[\frac{2\pi}{A(E)}\right]^{1/2}\cos[2\delta_0(E)-\pi/4], \tag{66}$$

where

$$A(E)=(2\mu E)^{1/2}r_0/\hbar, \tag{67}$$

r_0 is the location of the minimum of the interaction potential, and the functions $\beta_0(E)$, $\gamma_0(E)$, and $\delta_0(E)$ for various types of the potential are discussed in literature (see Ref. [4] and references therein).

The original Massey-Mohr cross section is [5,6]

$$\sigma_{mm}(E)=f_{mm}(s)\left(\frac{\mu C_s^2}{2E\hbar^2}\right)^{1/(s-1)}, \tag{68}$$

where

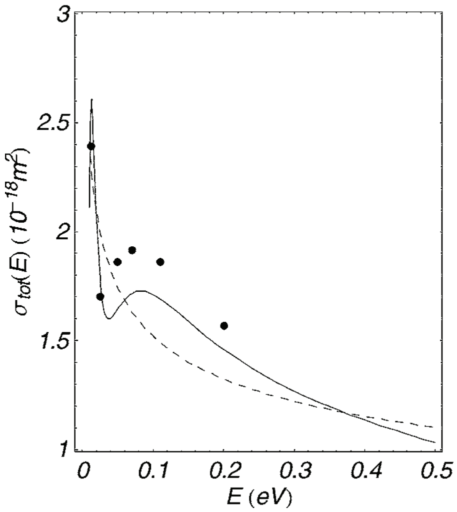

FIG. 11. The total cross sections $\sigma_{tot}(E)$ for low-energy H_2-Hg scattering when $s=6$. The solid line is the present ("corrected") cross section (65), and the dashed line is the ("original") cross section (68). The dots represent the calculated cross section of Ref. [38].

$$f_{mm}(s) = \pi\frac{2s-3}{s-2}[2p(s)]^{2/(s-1)}, \tag{69}$$

and $\Gamma(y)$ is a gamma function of argument y. For $s=6$, one has

$$\sigma_{mm}(E) = \left(\frac{4\pi^7\mu C_6^2}{E\hbar^2}\right)^{1/5}. \tag{70}$$

In the low-energy neutral-neutral collisions in field of a potential $C_n/r^n - C_6/r^6$, the ratio $\beta_0(E)/|\gamma_0(E)|^{1/2}$ can be given as [4]

$$\frac{\beta_0(E)}{|\gamma_0(E)|^{1/2}} \simeq 0.1816[G(E)][(E/D)^{1/20}], \tag{71}$$

where, as before, D is the well depth of the interaction potential, and $G(E)$ is a rather weak function of E when $0.1 \leqslant E/D \leqslant 100$ and the exponent n of the potential is between 4 and 12 [4]. Therefore the function can be approximated by the following power series when $4 \leqslant n \leqslant 12$ and $0.1 \leqslant E/D \leqslant 100$:

$$G(E) \simeq \xi_0 + \xi_1(E/D) + \xi_2(E/D)^2 + \xi_3(E/D)^3, \tag{72}$$

where $\xi_0=1.9632$, $\xi_1=-0.0428$, $\xi_2=0.0028$, and $\xi_3=-2.7\times10^{-5}$.

The phase shift δ_0 can be given in the form of the following expansion (of accuracy not worse than 0.5% when $E/D \geqslant 2$ and not worse than 3% when $1 \leqslant E/D \leqslant 2$)[37]:

$$\delta_0(E) \simeq [A(E)D/E][a_1 - A_1(E/D)^{-1} + A_2(E/D)^{-2}], \tag{73}$$

where the coefficients a_1, A_1, and A_2 are weak functions of the potential exponent n for the repulsive part of the interaction potential. Therefore one can assume in relationship (73) that the coefficients are constant (see discussion below) and equal to those for $n=8$ [37]: $a_1=0.4700$, $A_1=0.1644$, and $A_2=0.0821$.

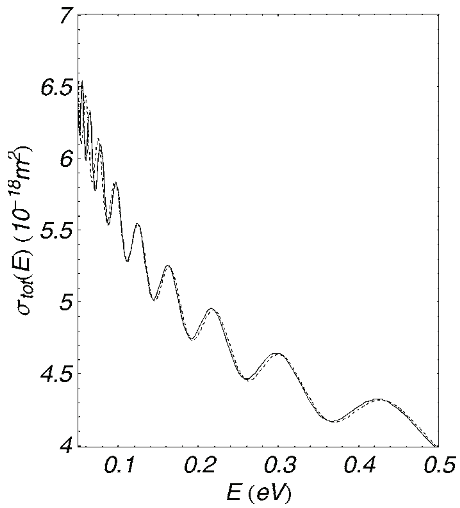

FIG. 12. The total cross section $\sigma_{tot}(E)$ [Eq. (65)] for the low-energy Na-Hg scattering when $s=6$. The solid and dashed lines are the cross sections calculated when using the phase shifts of the present work and those of Ref. [37], respectively (see the text).

To test the approach of this section, we calculated the total cross sections (65) for the H_2-Hg (Fig. 11) and Na-Hg (Fig. 12) collisions. (The H_2-Hg interaction is chosen to be studied here because some research on scattering is available in literature [38], and because the glory corrections $\Delta\sigma(E)$ for the interaction are larger than those in most of other collision systems (the reduced mass of the H_2-Hg system is small).

As seen in Fig. 11, the total cross section (65) for the H_2-Hg interaction (the solid line) shows similar energy dependence as the early partial wave calculations of Ref. [38] (the dots). The maximum difference (at $E\simeq 0.08$ eV) between the two cross sections is about 10%. [The potential used in Ref. [38] was Lennard-Jones (12-6) potential with $r_0=3.26\times10^{-10}$ m and $D=2.46\times10^{-21}$ J.]

The total cross section (65) for the Na-Hg interaction is calculated for two different sets of the coefficients occuring in the expansion (73). The first set of the coefficients is the one mentioned above ($a_1=0.4700$, $A_1=0.1644$, and $A_2=0.0821$), and the second set is that proposed for the Na-Hg interaction in Ref. [37] ($a_1=0.4700$, $A_1=0.1471$, and $A_2=0.0473$ at $r_0=4.72\times10^{-10}$ m and $D=8.79\times10^{-21}$ J.) The cross section calculated using the first set of the coefficients is shown in Fig. 12 as the solid line and the total cross section obtained using the second set of the coefficients is shown in the figure as the dashed line. The results shown in the figure suggest that, in general, it is justified to use the relationship (73) with the coefficients $a_1=0.4700$, $A_1=0.1644$, and $A_2=0.0821$ (see also Ref. [39]).

One should also add that the calculated locations of the extremes of the undulated total cross section $\sigma_{tot}(E)$ for the Li-Hg collision are close to the locations of the extremes found by Rothe and Veneklasen [40] who used an interaction potential with $r_0=2.82\times10^{-10}$ m and $D=7.80\times10^{-21}$ J.

The above discussion suggests that the total cross section (65) gives an acceptable description of most of the elastic small-angle scatterings of neutral particles at low impact energies.

VIII. THE SCATTERING PROBABILITIES

The "cumulative probability" $P_c(E,0 \leqslant \vartheta \leqslant \vartheta_c)$ [the probability of elastic scattering of two neutrals at impact energy E (when 0.05 eV$\lesssim E \lesssim$0.5 eV) into angles ϑ smaller than ϑ_c when $\vartheta_c \lesssim 3°$] is

$$P_c(E,0 \leqslant \vartheta \leqslant \vartheta_c) = \sigma_c(E,\vartheta_c)/\sigma_{tot}(E), \quad (74)$$

where

$$\sigma_c(E,\vartheta_c) = 2\pi \int_0^{\vartheta_c} I_B(E,\vartheta)\sin \vartheta d\vartheta, \quad (75)$$

where $I_B(E,\vartheta)$ is the differential cross section (45), and $\sigma_{tot}(E)$ is the total cross section (65) for the scattering.

Relationship (74) gives the following probability $P(E,\vartheta_1 \leqslant \vartheta \leqslant \vartheta_2)$ of elastic scattering of two neutrals at the impact energy E between 0.05 and 0.5 eV into an angle ϑ between ϑ_1 and ϑ_2 ($\vartheta_{1,2} \lesssim 3°$):

$$P(E,\vartheta_1 \leqslant \vartheta \leqslant \vartheta_2) = P_c(E,0 \leqslant \vartheta \leqslant \vartheta_c = \vartheta_2) - P_c(E,0 \leqslant \vartheta \leqslant \vartheta_c = \vartheta_1). \quad (76)$$

For $s=6$, the function (75) can be given as

$$\sigma_c(E,\lambda_c) = 2\pi q_0(E)\vartheta_0(E)\int_0^{\lambda_c} \sin(\vartheta_0\lambda)\Omega(\lambda)d\lambda, \quad (77)$$

where, as before, $q_0(E)$, $\vartheta_0(E)$, and $\Omega(\lambda)$ are given in relationships (53), (56), and (54), respectively, and

$$\lambda_c = \vartheta_c/\vartheta_0. \quad (78)$$

In small-angle scatterings, the values of the product $\vartheta_0\lambda$ are smaller than $(\vartheta_c)_{max} \simeq 3\pi/180 \simeq 0.05$. Therefore we expand $\sin(\vartheta_0\lambda)$ in expression (77) into a linear power series,

$$\sin(\vartheta_0\lambda) \simeq \vartheta_0\lambda, \quad (79)$$

so that the function (77) can be conveniently expressed by the following single-variable integral:

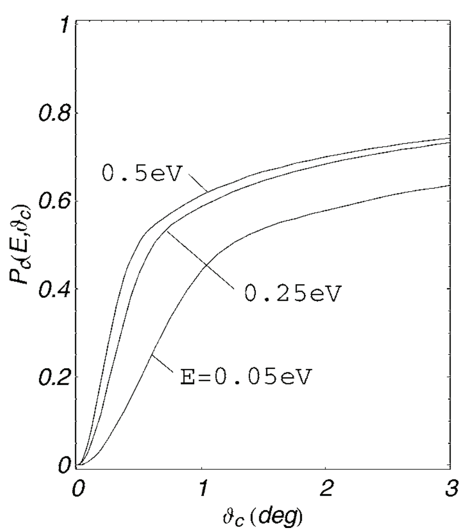

FIG. 13. The cumulative scattering probability $P(E,0 \leqslant \vartheta \leqslant \vartheta_c)$ [Eq. (74)] for the low-energy Li-Hg scattering when $s=6$.

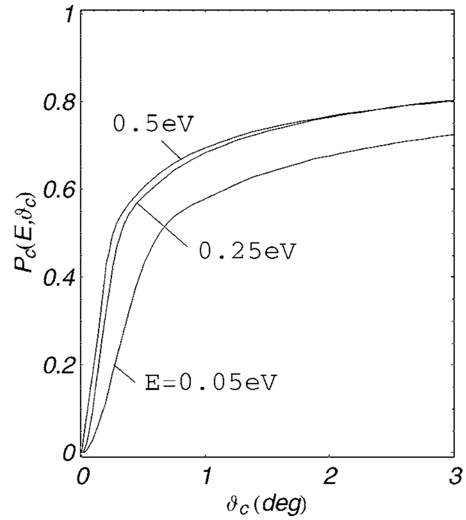

FIG. 14. The cumulative scattering probabilities $P(E,0 \leqslant \vartheta \leqslant \vartheta_c)$ [Eq. (74)] for the low-energy Na-Hg scattering when $s=6$.

$$\sigma_c(E,\lambda_c) = 2\pi q_0(E)\vartheta_0^2(E)\int_0^{\lambda_c} \lambda\Omega(\lambda)d\lambda. \quad (80)$$

In practical applications, the integral in relationship (80) can be estimated (using the Levenberg-Marquardt nonlinear fit) as

$$F(\lambda_c) = \int_0^{\lambda_c} \lambda\Omega(\lambda)d\lambda \simeq \{1 + a_0 \exp[-(b_0\lambda_c + c_0\lambda_c^{2/3} + d_0\lambda_c^{1/3})]\}^{-1}, \quad (81)$$

where $a_0=4.55305\times 10^5$, $b_0=2.06246$, $c_0=-11.10989$, and $d_0=21.44185$. [The approximation (81) is better than 10% in the considered ranges of the scattering angle ϑ and impact energy E but it should be used with caution when ϑ_c is very close to zero; $F(\lambda_c=0)=2.19\times 10^{-6}$.] Then, the function (80) can be approximated by

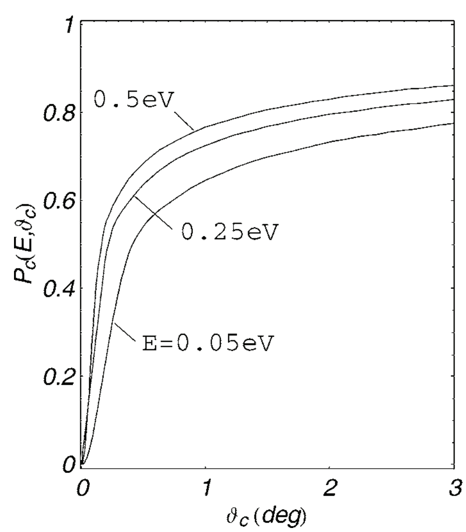

FIG. 15. The cumulative scattering probabilities $P(E,0 \leqslant \vartheta \leqslant \vartheta_c)$ [Eq. (74)] for low-energy K-Hg scattering when $s=6$.

$$\sigma_c(E,\lambda_c) \simeq 5.3718\left(\frac{C_6^2\mu}{E\hbar^2}\right)^{1/5} \times\{1 + a_0 \exp[-(b_0\lambda_c + c_0\lambda_c^{2/3} + d_0\lambda_c^{1/3})]\}^{-1}. \quad (82)$$

IX. ABSOLUTE SCATTERING PROBABILITIES FOR THE LI-HG, NA-HG, AND K-HG COLLISIONS

The cumulative probabilities (74) for low-energy, small-angle scattering in the Li-Hg, Na-Hg, and K-Hg collisions when $s=6$ are shown in Figs. 13–15, respectively. The results shown there confirm the importance of scatterings in center-of-mass angles of a few degrees in low-energy elastic collisions of neutral particles.

X. SUMMARY

The results discussed in the present work suggest that the "best" general and analytical expressions for studying low-energy ($0.05\ \text{eV} \lesssim E \lesssim 5\ \text{eV}$), center-of-mass binary scattering of neutral particles into small angles ($\vartheta \lesssim 3°$) are those given in relationships (45) (the absolute differential cross sections for the collisions), (65) [the collisions' total (integrated) cross sections], and (74) (the collisions' cumulative probabilities). The general accuracies of the relationships for a broad range of such neutral-neutral systems cannot be established at present since very few reliable measurements of scattering dynamics of the systems are available. However, it seems that the overall accuracy of the relationships should be acceptable (that is, not worse than about 10%) in many applications if the systems' interaction potentials are well-established.

ACKNOWLEDGMENTS

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