INVESTIGATIONS OF ELASTIC SCATTERING OF THE METASTABLE HELIUM ATOMS BY THE SODIUM ATOMS USING OPTICAL POTENTIAL MODEL

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The results of the pure quantum-mechanical calculation in the optical potential approach of integral cross sections in the wide collision energy region for the elastic scattering of singlet and triplet excited metastable helium atoms $He(2^{1,3}S)$ by sodium atoms $Na(3^2S)$ are presented. Low-energy (at the energies below 10 meV) structure of elastic cross sections was obtained. As an example, using the partial phase shifts and cross sections for the maxima 1 meV (for singlet case) and 0.4 meV (for triplet case) energies, the analysis of their origin is made. The comparison of the calculated Penning-ionization cross sections with the experimental and quasi-classical data is presented.

1. The investigation of elastic scattering of atomic particles is a part of a general trend in studying the properties of interatomic interaction and scattering characteristics. Precise experimental measurements of differential scattering cross sections and their energy dependences, as well as different integral cross sections may, together with theoretical calculations, also favour in solving the important problem of determining the optical potential (OP) of atomic interaction (see, e.g., [1,2]).

Up to date, the elastic collisions of ground state noble-gas atoms (Rg) were studied. A transition to the interaction of atoms, one of which being in the excited state (Rg^*), say, the metastable one, results in the interatomic potentials with large well depth reaching several millielectronvolts. Such values are due to the large polarizability of the elelectron shell in the excited atom. Recall that the asymptotic van der Waals behaviour of the interaction potential is $\sim - C_6 / R^6$, and the coefficient C_6, according to the Slater–Kirkwood formula [3], has a following form

$$C_6 = \frac{3}{2} \frac{\alpha_1 \alpha_2}{\sqrt{\alpha_1} + \sqrt{\alpha_2}} \text{ (a.u.)},$$

where $\alpha_{1,2}$ are the static polarizabilities of interacting atoms.

Further expansion of studies to the interaction of excited Rg^* atoms with metal atoms (M) of alkali, alkaline-earth, and rare-earth elements, taking into account their large polarizabilities, means that the interaction will also be characterized by considerable potential well depths. Thus, from the fundamental view-point, the studies of the characteristics of elastic atom-atom scattering described by the interaction potential with large depth are of specific interest. Study of this process at low collision energies will, most likely, be characterized by the resonance features related to the formation of temporary bound (compound) states of quasi-molecular (Rg^*M) type. In this case, the most general scattering characteristics are the integral ones, i.e. total, elastic, and ionization scattering cross sections. Note that elastic scattering of Rg^* atoms by alkali-earth (and rare-earth) atoms may lead to excitation of the positive ion produced, which complicates essentially the description of the process (an additional channel arises).

Low collision energy as compared to the potential well depth requires, in our opinion, the theoretical method to be mainly quantum-mechanical one, while usually various modifications of semiclassical approximation are used. Hence, the objective of this work is to present a brief survey of papers dedicated to interaction OP at elastic collisions of excited rare-gas atoms with metal atoms, quantum-mechanical calculation of scattering phases in the OP approximation and, based on this, determination of integral cross sections within a wide range of meV and thermal energies, and theoretical description of their peculiarities in the strong interactions of $He(2^{1,3}S)$ and $Na(3^2S)$ atoms. Scattering phase calculations were carried out by the method of phase functions [4 – 6] with complex OP [7]. The

theoretical results of calculations of the integral characteristics presented below have a preliminary character.

Such calculations allow the model notions used for defining OP for atoms in various excited states to be checked. The use of the quasi-classical approximation for taking into account a large number of partial waves at quite large energies (e.g., above 50 meV) will enable one to distinguish better and clarify the quantum-mechanical and semiclassical aspects of the scattering process. Resulting total, differential, diffusion, and viscosity cross sections may be used in various dynamical models of gas and plasma.

2. Interaction of a metastable $He(2^{1,3}S)$ atom with a ground-state $Na(3^2S)$ atom is characterized by two total spin values of quasi-molecular terms $^{-}$ 1/2 and 3/2. Singlet helium atom scattering occurs via one doublet $^2\Sigma^+$ quasi-molecular term, whereas this takes place for the triplet state via two terms $^{-}$ the doublet $^2\Sigma^+$ (statistical weight 2/6) and quartet $^4\Sigma^+$ (4/6) ones. Note that the doublet-term interaction is described by the complex OP, while the quartet-term one $^{-}$ by the real OP. The real part OP via doublet terms was obtained in [7] in the interacting configuration approximation for a $NaHe^*$ molecule with the use of fitting to the correct asymptotic behaviour $^{-}$ the van der Waals potential. Imaginary parts of these OP (i.e., autoionizing widths) were obtained using the Stieltjes moment method with continuum representation discretization for the $e + NaHe^+$ system in the (L^2) space.

The theoretical methods of obtaining the *ab initio* OP for the description of interatomic interaction in the 'metastable Rg atom + metal M atom“ system are available now considering the above system as the collisional autoionizing complex Rg^*M [3, 7 $^{-}$ 9]. The obtained OP are used for the detailed description of elastic scattering and analysis of characteristics of electron spectra for the Penning-ionization (PI) process.

In [7], OPs for singlet and triplet metastable helium atom scattering by sodium atom were obtained by calculating in terms of resonance electron energy and autoionizing width, and also used to calculate differential cross sections (DCS) in semiclassical approximation and determine PI cross sections within a wide thermal energy range from 10 to 1000 meV. In [8], based on the same assumptions, *ab initio* OPs were obtained for interaction of helium metastables with H, Li, Na atoms. The similar technique was applied in [3] to study interactions of helium metastables with Mg, Ca, Sr, and Ba atoms. In [9], the potential well values of the real part of OP derived from high-resolution PI electron spectra were generalized for the many Rg^*M systems (Rg = He, Ne, Ar, Kr, Xe, M = Li, Na, K, Rb, Cs, Mg, Ca, Sr, Ba, Yb, Hg).

One more possibility to obtain OP, similarly to the case of $He(2^1S) + Na(3^2S)$ scattering at 52, 92, 132, 188, and 207 meV energies and laboratory scattering angles $\theta_L = 5 \div 105°$ [2], is fitting of calculated DCS to the experimental one (the so-called direct approach to the solution of the reverse scattering problem) by χ^2 method. In this paper, the semiclassical approximation is used, the real part of the OP has the form of a modified double Morse potential [1], and the imaginary one is taken as a simple exponent.

In [10], the phase functions method was used in quantum-mechanical calculations of scattering phases, DCS, and other characteristics of $He(2^1S) -$ $- Na(3^2S)$ scattering at 68 meV, while, in [11, 12], based on OP from [2], the theoretical phase analysis of this process was carried out at 52, 80, and 92 meV. Similarly, in [6] with OP taken from [7], the same characteristics were calculated for the $He(2^{1,3}S) -$ $- Na(3^2S)$ case. The obtained DCS were used to interpret the measured summary DCS for these processes [13]. In [14], OPs for the $He(2^3S) -$ $- Na(3^2S)$ pair (doublet and quartet terms) were used for semiclassical calculation of PI cross section and of such pure quantum-mechanical scattering characteristic for triplet helium as the exchange cross section within the $\sim 10 - 200$ meV energy range. OP for attractive quartet term [14] was also used in [6] for the semiclassical evaluation of the quartet addends to the total and elastic cross sections at 68 meV. These addends are 2.5 times larger than those for doublet one. Note again that the interaction via the quartet term does not contribute to the PI cross section.

We used the optical potentials [7] (for two cases $^{-}$ singlet and triplet excited metastable states of helium) of He atom scattering by Na. Principal characteristics of these OPs for 2^1S (2^3S)-state of He are as follows: real parts of doublet OP have a strong repulsion at $R \le 0.2a_0$ (for example: $V(0.1a_0) =$ $= 227.97$ a.u. (484.09 a.u.), $V(0.2a_0) = 50.062$ a.u. (87.715 a.u.)); zero value at $R_0 \approx 5.75a_0$ ($4.45a_0$); minimal value $V_{Rm} = -300$ meV at $R_m = 7.35a_0$ ($V_{Rm} = -740$ meV, $R_m = 5.85a_0$); asymptotic behaviour $-C_6/R^6$, $C_6 = 3660$ a.e. (2220 a.e.), that approximately 'begins“ at $R_a = 8.22a_0$ ($6.27a_0$). Imaginary parts of OP [7] describing the PI process are characterized by nearly exponential behaviour at $R \ge 5a_0$ with some deflection from it at $R < 5a_0$. As this takes place, beginning at $6a_0$, the imaginary part for the 2^1S-state decreases more rapidly than for the

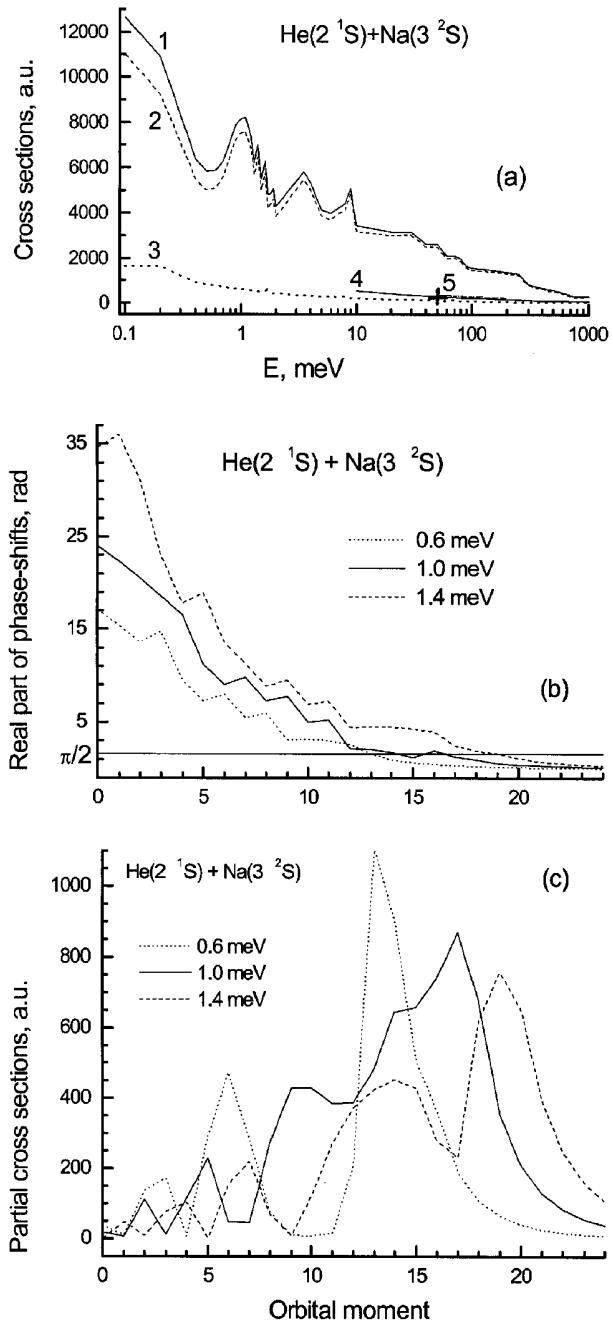

Fig.1. Integral cross sections (*a*), real part of partial phase shifts (*b*) and partial cross sections (*c*) for $He(2^1S)$ – $Na(3^2S)$ elastic scattering. *a* – present result: total (*1*), elastic (*2*) and Penning-ionization (*3*); Penning-ionization: quasi-classical theory (*4*) [7], (*5*) [2]; experiment (+) [17]

2^3S-state (for example, the triplet part is 5 times greater than the singlet one at $R = 11a_0$).

3. Quantum description of the relative motion of atoms in the Born – Oppenheimer adiabatic approach can be described by Schrodinger equation with the complex OP – $V_{\text{opt}}(R)$ (center-of-mass system, atomic units: $h = m_e = e = 1$) (see [6, 10])

$$\left[-\frac{1}{2\mu}\nabla_R^2 + V_{\text{opt}}(\mathbf{R}) - E \right] \Psi(\mathbf{R}) = 0, \qquad (1)$$

where $V_{\text{opt}}(\mathbf{R}) = V_R(\mathbf{R}) + i\,V_I(\mathbf{R})$, E is the kinetic collision energy, μ is a reduced mass (6214 a.u. for He–Na), R is an internuclear distance.

The system of equations for the complex phase functions $\delta_l(E, R) = \varepsilon_l(E, R) + i\,\bar{\eta}_l(E, R)$ is obtained from (1) [4, 5] and has a form

$$\frac{d\varepsilon_l}{dR} = -\frac{1}{4k\,\eta_l}\{V_R[(1+\eta_l)^2(j_l\cos\varepsilon_l - n_l\sin\varepsilon_l)^2 -$$

$$-(1-\eta_l)^2(j_l\sin\varepsilon_l + n_l\cos\varepsilon_l)^2 +$$

$$+ 2V_I(1-\eta_l^2)(j_l\cos\varepsilon_l - n_l\sin\varepsilon_l)(j_l\sin\varepsilon_l + n_l\cos\varepsilon_l)\},$$

$$\frac{d\eta_l}{dR} = \frac{1}{2k}\{V_I[(1+\eta_l)^2(j_l\cos\varepsilon_l - n_l\sin\varepsilon_l)^2 -$$

$$-(1-\eta_l)^2(j_l\sin\varepsilon_l + n_l\cos\varepsilon_l)^2] -$$

$$-2V_R(1-\eta_l^2)(j_l\cos\varepsilon_l - n_l\sin\varepsilon_l)(j\sin\varepsilon_l + n_l\cos\varepsilon_l)\}, \qquad (2)$$

with the initial conditions

$$\varepsilon_l(E, 0) = 0, \quad \eta_l(E, 0) = 1, \qquad (3)$$

where $\eta_l(E, R) = \exp(-2\,\bar{\eta}_l(E, R))$; $k^2 = 2\mu E$, and $j_l \equiv j_l(kR)$, $n_l \equiv n_l(kR)$ are the Riccatti – Bessel functions. Real $\varepsilon_l(E)$ and imaginary $\bar{\eta}_l(E)$ parts of the partial scattering phase shifts $\delta_l(E)$ are obtained from the corresponding phase functions

$$\varepsilon_l(E) = \lim \varepsilon_l(E, R), \quad \bar{\eta}_l(E) = -\frac{1}{2}\ln\lim \eta_l(E, R),$$

at $R \to \infty$. (4)

The solution of system (2) with condition (3) was carried out numerically by methods described in detail in [6, 10].

It should be noted here that the analytic expressions for OP [2] were obtained in [10] for these parts of phase functions at low R ($kR \le 0.05$). From these expressions, the strong dependence of the real and imaginary values of phase functions on the orbital momentum, wave vector, and potential parameters follows.

The use of the phase functions method is quite promising due to the fact that these functions allow the interaction potential to be 'scanned“. Recall that, by definition, this function at a certain point R is the phase of scattering by the corresponding potential cut at the same point. Therefore, this method allows one to trace the formation of the whole scattering phase shift in different spatial domains of given potential [4, 5].

The scattering phases calculated by us were used to obtain the following integral-type cross sections elastic scattering σ_{el}; absorption (Penning-ionization) σ_i; total σ [15, 16]]:

$$\sigma_{el}(E) = \sum_l \sigma_l(E), \quad \sigma_l(E) = \frac{g\pi}{k^2}(2l+1)|S_l - 1|^2,$$

$$\sigma_i(E) = \frac{g\pi}{k^2}\sum_l (2l+1)(1 - |S_l|^2),$$

$$\sigma(E) = \frac{2\pi}{k^2}\sum_l (2l+1)(1 - \mathrm{Re}\, S_l) = \sigma_{el}(E) + \sigma_i(E),$$

$$S_l = \exp[2i\,\delta_l(E)]. \qquad (8)$$

For doublet terms in the case of $He(2^{1,3}S) + Na(3^2S)$ scattering, the statistical weights g are 1 for singlet and 1/3 for the triplet He atoms.

4. In Figs. 1, 2, we present the calculated scattering characteristics for singlet and triplet helium atoms impacting on a sodium atom. Our calculations were only quantum-like, and about 50 (at small) and 150 (at large energies) partial waves were taken into account. As follows from Figs. 1,*a*, 2,*a*, our PI cross sections are characterized by the lack of structure and by a quite monotonous behaviour. From the figures, we also see good agreement of the above cross sections with a few experimental values and the quasi-classical [2, 7, 14] curves: for singlet case at $E = 50$ meV – $214a_0^2$ (± 100%) [17], and for triplet at $E = 40$ meV – $114a_0^2$ (+ 5%, – 10%) [18]; at 50 meV – $86a_0^2$ (± 100%) [17]. Note that our curves $\sigma_i(E)$ systematically lie slightly below the quasi-classical values [2] obtained with OP recovered by experimental DCS and with OP [7, 14] testifying in favour of our quantum calculation.

The well-defined gross structure at very small energies, lower than 10 meV, in the total and elastic cross section exists and owes its existence to the quantum-mechanical description at small energies: for singlet scattering at 1, 3.5, 9 meV and for triplet scattering at 0.4, 0.9, 2, and ~ 6.5 meV. It follows from Figs. 1,*a*, 2,*a* and (8) that the structure in total cross sections is due to elastic cross sections, since PI ionization cross sections are characterized by the above monotonous behaviour.

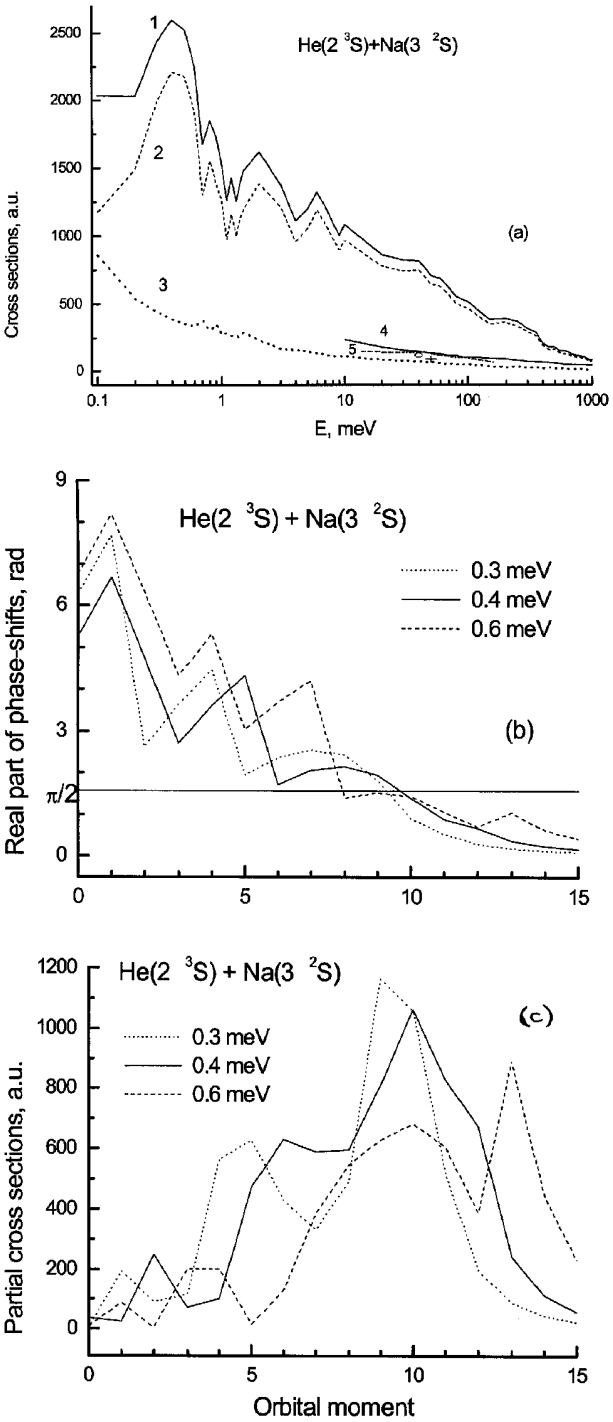

Fig.2. The same as in Fig.1 for $He(2^3S)$ – $Na(3^2S)$ elastic scattering. *a* – present result: total (*1*), elastic (*2*) and Penning-ionization (*3*); Penning-ionization: quasi-classical theory (*4*) [7], (*5*) [14]; experiment (+) [17], (o) [18]

It seems interesting to find the ratio of ionization cross sections $q = \sigma_i(He(2\,^1S))/\sigma_i(He(2\,^3S))$ at different collision energies. In [8], it is stated that

this ratio depends weakly on the energy. Recall, that it should be 3, corresponding to that of statistical weights of spin-allowed collisions. According to experiments, at 50 meV $q = 2.5$ [17], at 70 meV 2.8 (± 30%) [8] and 3.1 (± 30%) [19]. Our values of $q(E)$ at some energies are as follows: 1.9(0.1), 2.4(0.5), 2.2(1), 2.0(5), 2.1(10), 2.1(50), 2.0(68), 2.1(70), 2.0(100), 2.4(500), and 2.2(1000). As is seen, the theoretical values are systematically less than 3 and this is a general trend in calculations (see also [6]).

$He(2\,^1S) + Na(3\,^2S)$ scattering. The real part of the partial phase shifts and cross sections from Fig. 1,*b*,*c* is used to explain a feature near 1 meV for singlet helium scattering. The maximum value of the elastic cross section at this energy is reached due to the partial cross sections contribution at $l = 8 \div 19$ (in this case, the cross section varies from ~ 300 to $850a_0^2$). The real part of the phase shifts has $5\pi/2$ or $\pi/2$ values for these orbital momenta at the 1 meV energy, and the addends to the respective partial cross sections are maximal.

Energy dependences of the partial phase shifts $\delta_{16,17,18}(E)$ pass the value of $\pi/2$ at $E = 0.9$, 1.0, and ~ 1.15 meV, respectively. This gives a maximum of σ_{17} at 1.0 meV and a such a behaviour of the scattering phase allows one to state that the feature in σ_{el} at this energy is of resonance nature.

$He(2\,^3S) + Na(3\,^2S)$ scattering. For the triplet helium scattering, from Fig. 2,*a*, the maximum value of the elastic cross section at the 0.4 meV energy is due to the partial cross sections contribution at $l = 5 \div 12$ (cross sections vary from ~ 500 to $\sim 1100a_0^2$), as seen from Fig. 2,*b*,*c*. The real parts of the phase shifts are close to $3\pi/2$ or $\pi/2$ values for these orbital momenta at the 0.4 meV energy, and the respective addends from partial cross sections at this energy are larger than those from the neighboring ones for the 0.3 and 0.6 meV energies. Nevertheless, it is seen from Fig. 2,*b*,*c* that the partial cross sections in this orbital momenta interval at 0.3 and 0.6 meV are similar and, thus stimulate the maximum in the cross section at 0.4 meV.

The energy dependences of the partial phase shifts $\delta_{8,9}(E)$ pass the value of $\pi/2$ at $E \approx 0.2, 0.3$ meV, respectively, and $\delta_{10}(E)$ reaches this value at ~ 0.5 meV. This gives a maximum of σ_{10} at 0.4 meV and such a behaviour of the scattering phase allows one to state that the feature in σ_{el} at this energy is also of a resonance origin.

Some concluding remarks can be made. The quantum notions used in the calculations for the system of strongly interacted atomic particles Rg^*M in the OP approximation, when the system is treated as the autoionizing complex, describe correctly the characteristics of elastic scattering at the given energy. PI cross sections calculated by us with the use of above OPs agree quantitavely well with the available experimental data. The energy dependence of these cross sections is similar to the behaviour of the revelant semiclassical values and goes below them.

The peculiarities in the total cross sections are the result of only the behaviour of elastic cross sections. These peculiarities are due to the fact that the quasi-molecular shape resonances at these energies do exist. This structure requires a good explanation within the framework of a more complete phase analysis. The initial (threshold) behaviour of the total (elastic) cross sections for the singlet and triplet cases is very different and may be due to the respective optical potential behaviour.

In future, one needs to perform the quasi-classical calculations of the highest partial waves and their addend to the integral cross sections, to consider the quantum-mechanical spin exchange process for the priplet helium scattering (in view of the doublet and quartet term interaction), and to explain other peculiarities in both cases of excited helium atom scattering.

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