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Collisional quenching of the pionic helium long-lived states

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MOTIVATION

Recently laser-induced transition

$$(n = 17, l = 16) \rightarrow (n = 17, l = 15)$$

in pionic helium $(\pi^{-}\,{}^{4}\mathrm{He}^{+})_{nl}$ was observed for the first time (M. Hori, *et al.*, Nature **581**, 2020, 37).

A possibility of the further precision laser spectroscopy of this system depends, in particular, on the stability of the states against the quenching by collisions with the medium atoms. Stark transitions between the highly excited states in the collisions

$$(\pi^{-}\mathrm{He}^{+})^{*}_{nl} + \mathrm{He} \rightarrow (\pi^{-}\mathrm{He}^{+})^{*}_{nl'} + \mathrm{He} \quad (l' \neq l), \tag{1}$$

can be expected as the most probable due to a small difference between the initial and final inner energies.

THEORETICAL APPROACH: SCHEME

- Step 1: In order to obtain an interaction between the colliding systems $((\pi^- \text{He}^+)^*_{nl} + \text{He})$ we calculate the Potential Energy Surface (PES) of the three electrons in the field of three heavy particles (two α-particles and π^-).

- Step 2: Solution of the coupled-channels equations with the obtained PES and calculations of the cross sections and transitions rates of the Stark transitions (1).

- Step 3: Kinetics of the pion transitions up to nuclear absorption.

POTENTIAL ENERGY SURFACE
and
INTERACTION BETWEEN $(\pi^-\mathrm{He}^+)^*_{nl}$ AND He ATOMS

Heavy particles (helium nuclei and pion) are slow ($v_{hp} \ll v_e$), $\therefore$ electronic variables can be separated out within adiabatic approximation reducing the problem to the 3-body system of heavy particles with an effective adiabatic interaction

$$V(r,R,\cos\theta) = \frac{4}{|\mathbf{R}+\nu\mathbf{r}|} - \frac{2}{|\mathbf{R}-\lambda\mathbf{r}|} + E_e(r,R,\cos\theta) - \epsilon_e(r) - E(\mathrm{He}), \tag{2}$$

where r is the distance from the nucleus a to π^-, R is the distance from the center of mass $\pi^- a$ to the nucleus b, and θ is the angle between $\mathbf{r}$ and $\mathbf{R}$, $\lambda = M_a/(M_a + m_\pi)$, $\nu = 1 - \lambda$, $E_e(r,R,\cos\theta)$ is the total energy of 3 electrons in the field of 3 heavy particles, $E(\mathrm{He})$ is the inner energy of the isolated He atom, and $\epsilon_e(r)$ is the energy of electron in the field of two heavy particles (a and π^-) separated by the distance r.

METHOD OF THE PES CALCULATION

The energies $E_e(r, R, \cos\theta)$, $\epsilon_e(r)$ and E(He) were calculated within unrestricted Hartree-Fock approximation taking into account (e-e)-correlations in the second-order perturbation theory. An extended set of molecular basis functions aug-cc-pV5Z was used, taking into account correlations and valence polarization. Electronic orbitals were centred on a and b nuclei. Numerical calculations were performed using an original program based on the RI ("resolution of identity") method for computing of the integrals of electron-electron interactions.

(PES for this system was calculated earlier by B. Obreshkov and D. Bakalov, Phys. Rev. A **93**, 2016, 062505, however no data for the PES were published, therefore we done independent calculations.)

Total energy E_{nl} of the isolated (π^-He$^+$) atom in the adiabatic approximation is the eigenvalue of the Hamiltonian

$$H_\pi = T_r - \frac{2}{r} + \epsilon_e(r) \tag{3}$$

(n,l)	Korobov	Adiabatic Appr.
(16,15)	-2.82854939373(4)	-2.82776
(17,14)	-2.70984178(2)	-2.70806
(17,15)	-2.68542722(2)	-2.68441
(17,16)	-2.65751243850171	-2.65722

Multipole decomposition

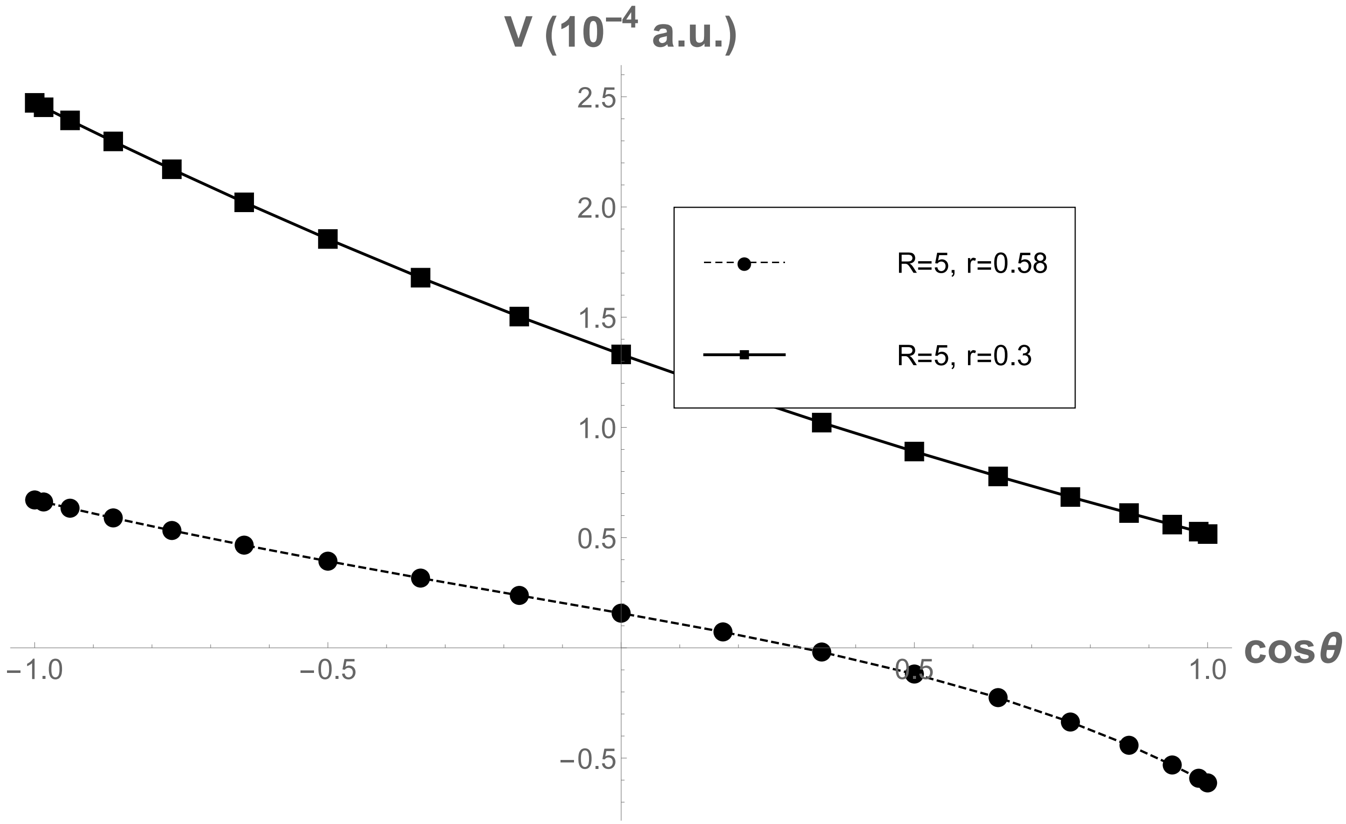
To highlight the angular dependence of $V(r, R, \cos\theta)$ we expand it in a series of Legendre polynomials

$$V(r, R, \cos\theta) = \sum_{k=0}^{\infty} V^k(r, R) P_k(\cos\theta), \tag{4}$$

where

$$V^k(r, R) = (k + 1/2) \int_{-1}^{1} V(r, R, t) P_k(t) dt. \tag{5}$$

The performed calculations show that $V(r, R, \cos\theta)$ at $R > r$ depends smoothly on $\cos\theta$, therefore for a consideration of thermal collisions we can restrict the series (4) by the lowest terms.



Angular dependence of PES for the interaction between (π^{-}He^{+}) and ordinary ^{4}He atom at $r = 0.3$ and 0.58, $R = 5$.

Coupled channels approach

Basis set: $|j\rangle \equiv |nl, L : JM\rangle = u_{nl}(r)\,(Y_l(\Omega_r) \otimes Y_L(\Omega_R))_{JM}$.
We restrict the set by the states with a fixed n. Total wave function:
$\boldsymbol{\Psi}_i(\mathbf{R}, \mathbf{r}) = \sum_{lL} |j\rangle \psi_{ji}(R)/R$.
System of coupled channels equations:

$$\psi''_{ji}(R) + \left[k_j^2 - L_j(L_j+1)/R^2\right]\psi_{ji}(R) = 2m\sum_k V_{jk}(R)\psi_{ki}(R)$$

$$k_j^2 = \begin{cases} 2m(E - E_{nl}) & \text{(real) if } l \geqslant 2, \\ 2m(E - E_{nl} + \epsilon_{nl} + \frac{\mathrm{i}}{2}\Gamma_{nl}) & \text{(complex) if } l_j \leqslant 1. \end{cases}$$

$\therefore$ Boundary conditions in the channels with $l_j, l_i \geqslant 2$ are standard, but in the channels with $l_j \leqslant 1$, $l_i \geqslant 2$ $\psi_{ji}(R) \rightarrow\sim \exp(-\mathrm{Im}(k_j)R)$, and $\psi_{ji}(R) = 0$ at $l_i \leqslant 1$.

Matrix elements

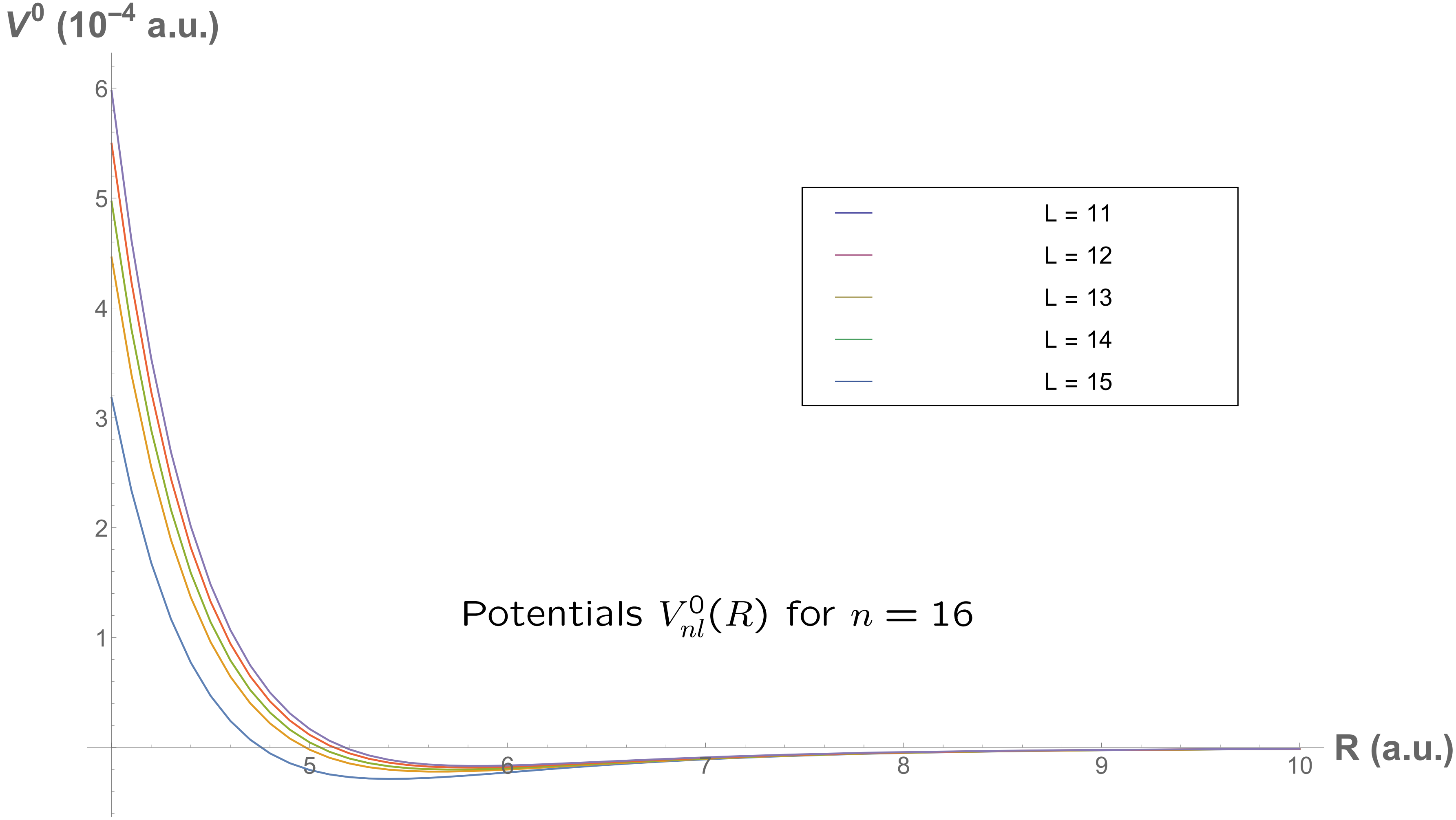
Using the multipole decomposition, matrix elements of $V(\mathrm{r}, \cos\theta, \mathrm{R})$ are reduced to the radial integrals:

$$\langle nl', L' : JM | V(\mathrm{r}, \cos\theta, \mathrm{R}) | nl, L : JM \rangle = \delta_{ll'} \delta_{LL'} V^0_{nl}(R) + \langle l'L' : JM | \cos\theta | lL : JM \rangle \cdot V^1_{nl,nl'}(R) + \ldots \quad (6)$$

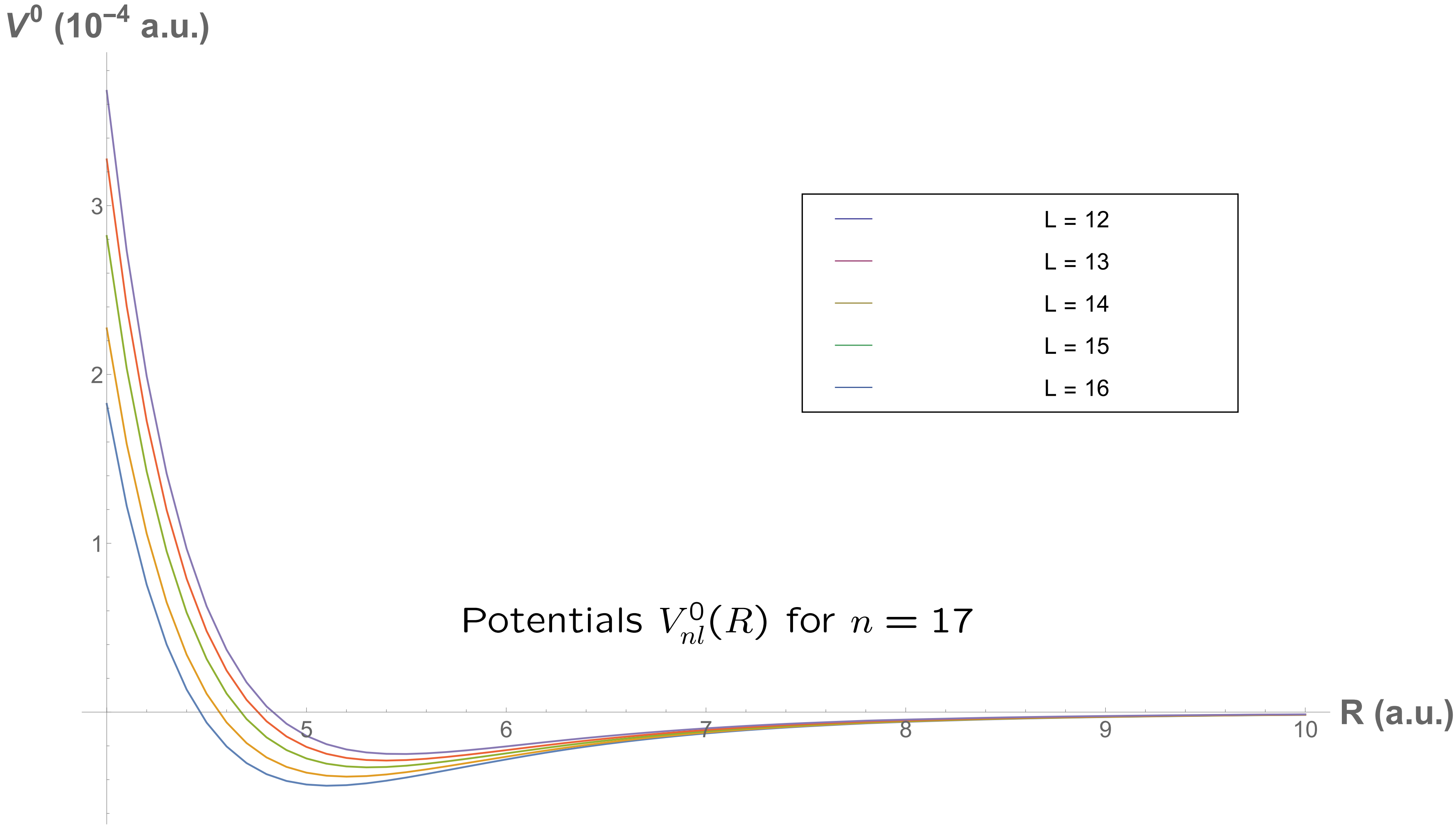
where

$$V^0_{nl}(R) = \int_0^\infty u^2_{nl}(r) V^0(r, R) r^2 dr$$

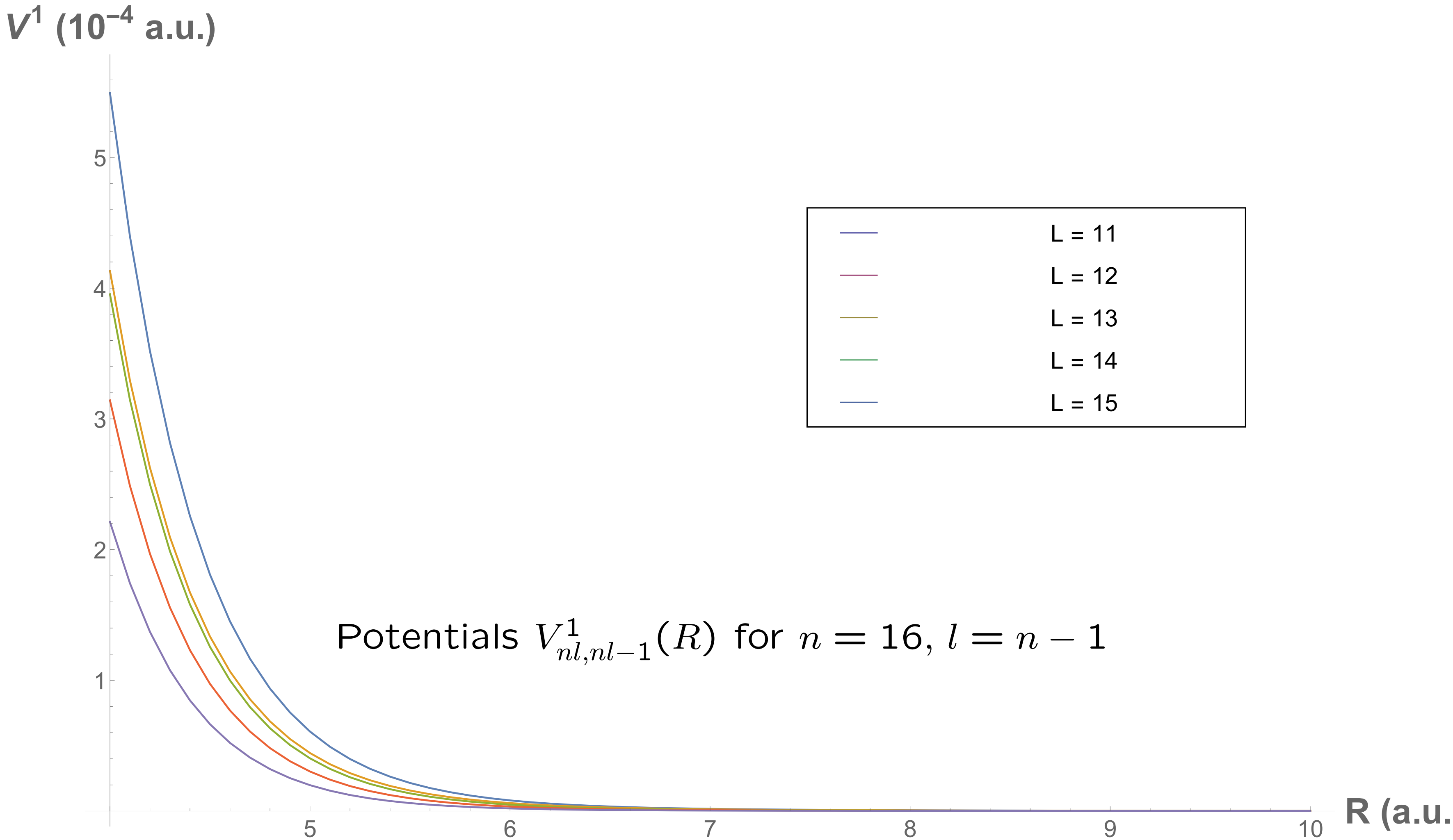
$$V^1_{nl,nl'}(R) = \int_0^\infty u_{nl}(r) u_{nl'}(r) V^1(r, R) r^2 dr \quad (l' = l \pm 1)$$



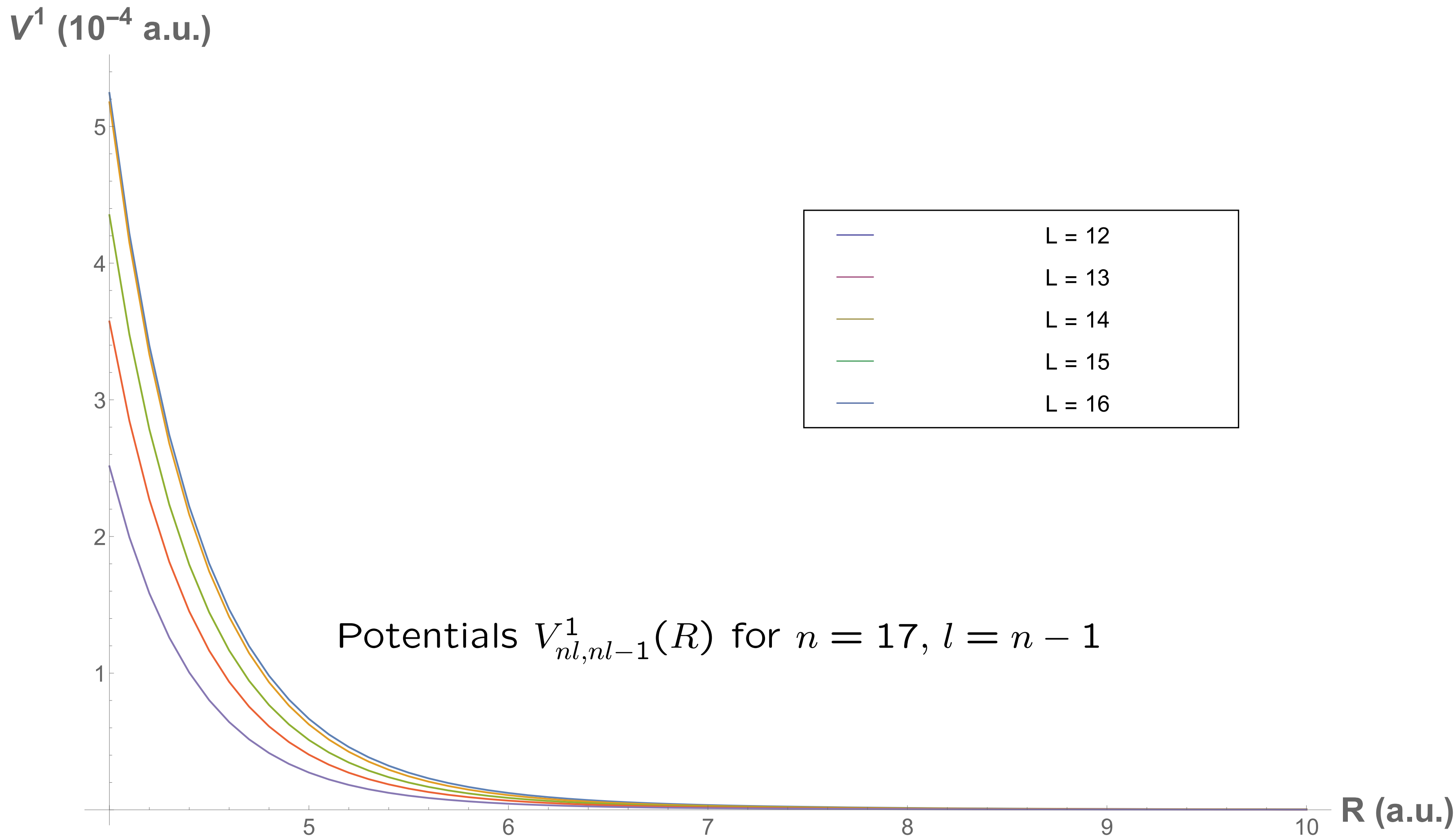
V^0 (10^{-4} a.u.)
6
5
4
3
2
1
5
6
7
8
9
10
R (a.u.)
L = 11
L = 12
L = 13
L = 14
L = 15
Potentials $V_{nl}^0(R)$ for $n = 16$



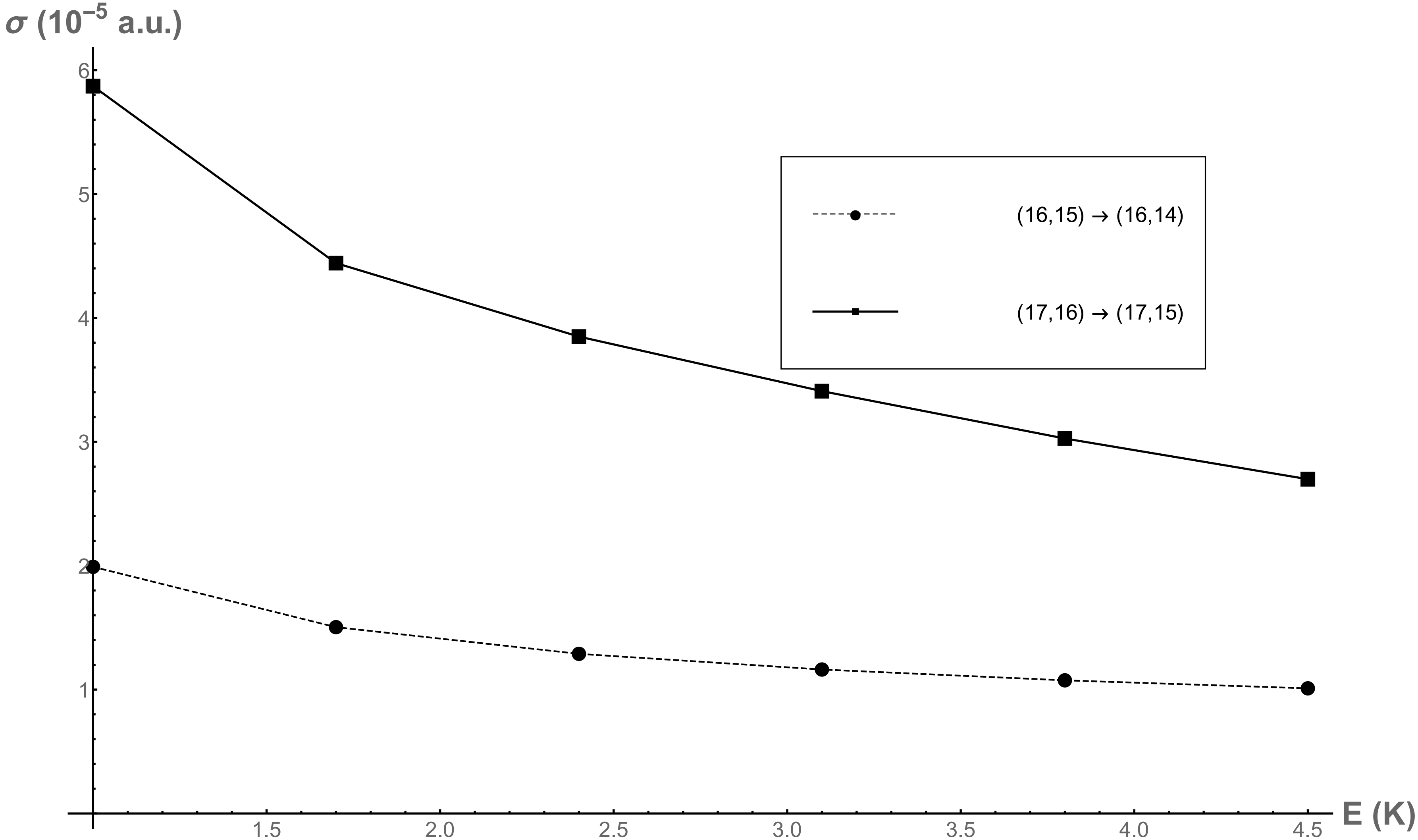
V^0 (10^{-4} a.u.)
3
2
1
5
6
7
8
9
10
R (a.u.)
L = 12
L = 13
L = 14
L = 15
L = 16
Potentials $V^0_{nl}(R)$ for $n = 17$



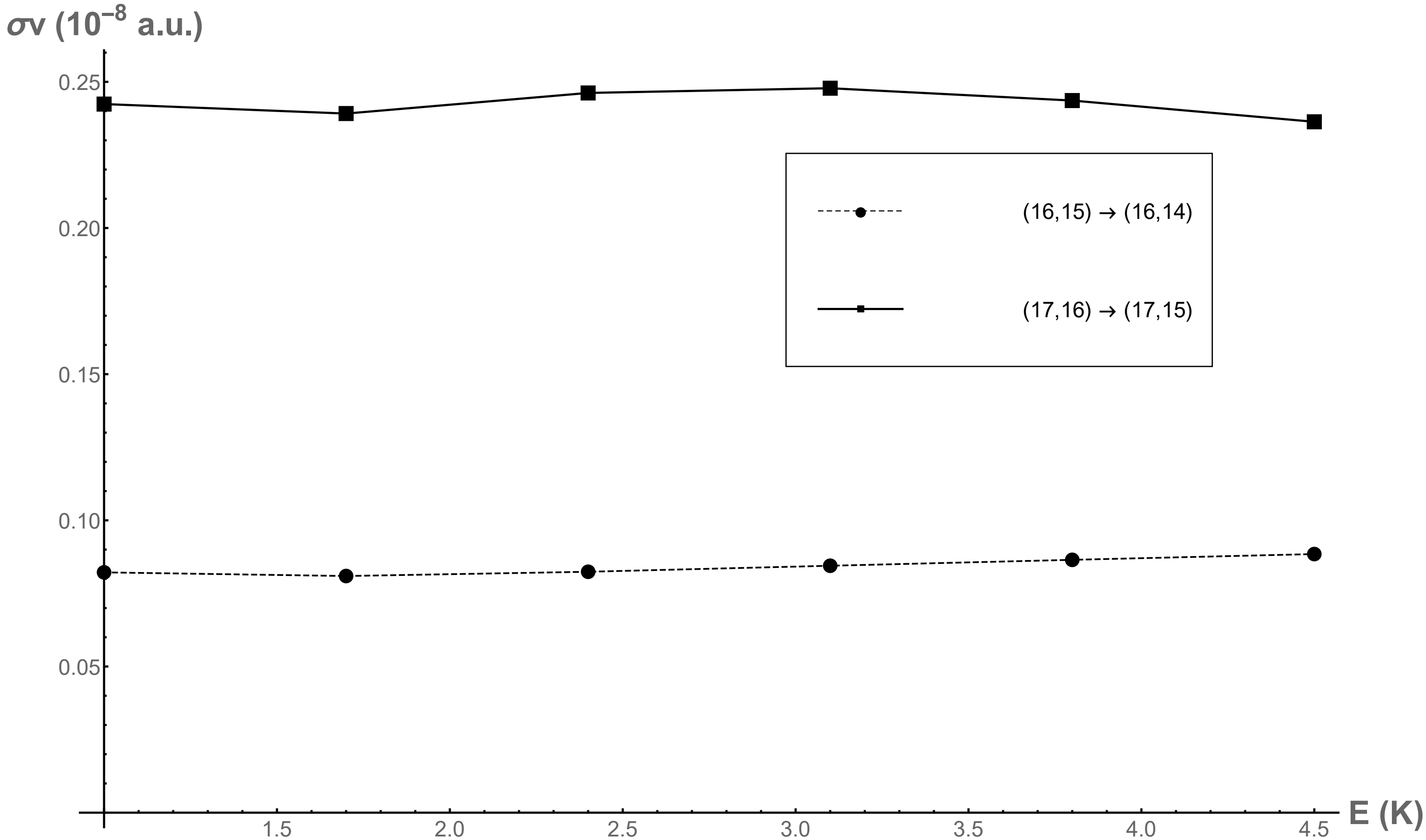
Potentials $V^1_{nl,nl-1}(R)$ for $n = 16$, $l = n - 1$



V^1 (10^{-4} a.u.)
5
4
3
2
1
5
6
7
8
9
10
R (a.u.)
L = 12
L = 13
L = 14
L = 15
L = 16
Potentials $V^1_{nl,nl-1}(R)$ for $n = 17$, $l = n - 1$



Cross sections of the transitions $n,\, l = n-1 \rightarrow n\, l' = l-1$



Reduced rates $\sigma \cdot v$ of the transitions $n,\, l = n-1 \to n\, l' = l-1$

Conclusion

Systematic calculations of the cross sections and transition rates for the $(\pi^-\text{He}^+)$ – He collisions are still in progress, therefore we can make only preliminary remarks on these values. It is seen from the Figs. above that Stark cross sections $(n, l = n-1 \rightarrow n, l-1)$ decrease as $\sim 1/v$ with increasing energy in the range E=1-4.5 K, and corresponding reduced transition rates (σv) are constants in this region.

The cross section of the $(17, 16 \rightarrow 17, 15)$ transition is more than that one of the $(16, 15 \rightarrow 16, 14)$ transition by about 3 times.

Using the conversion constant $a_0^2 v_a = 6.126 \cdot 10^{-9}\,\text{cm}^3/\text{s}$ (from atomic to common units) and the density $\rho = 2.18 \cdot 10^{22}\,\text{cm}^{-3}$ of a superfluid He at T=1.7 K we estimate a rate of collisional transition from the state (17,16) as $\lambda_{17,16} \simeq 3.2 \cdot 10^5\,\text{s}^{-1}$, or lifetime with respect to quenching $\tau_q \simeq 3 \cdot 10^{-6}$ s.