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Improved study of the 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; M. Hori, *et al.*, Few-Body Syst.**62**, 63 (2021)).

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 $((\pi^- \mathrm{He}^+)^*_{nl} + \mathrm{He})$ 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.

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.)

Matrix elements

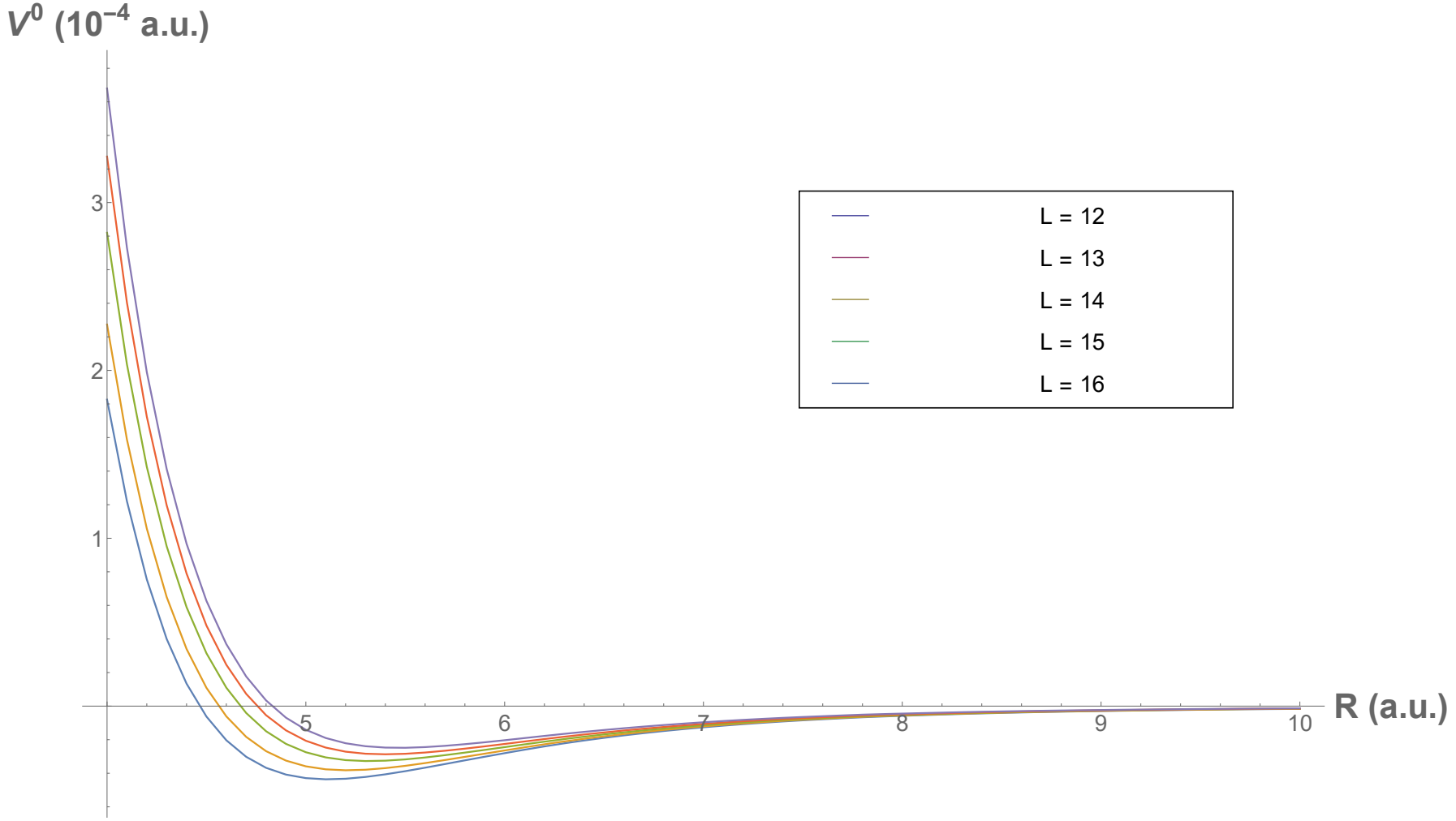
Using the multipole decomposition, matrix elements of $V(\mathrm{r}, \cos\theta, \mathrm{R})$ are reduced to the radial integrals:

$$\langle nl', L' : JM|V(\mathrm{r}, \cos\theta, \mathrm{R})|nl, L : JM\rangle = \delta_{ll'}\delta_{LL'}V^0_{nl}(R) + \langle l'L' : JM|\cos\theta|lL : JM\rangle \cdot V^1_{nl,nl'}(R) + \ldots \quad (2)$$

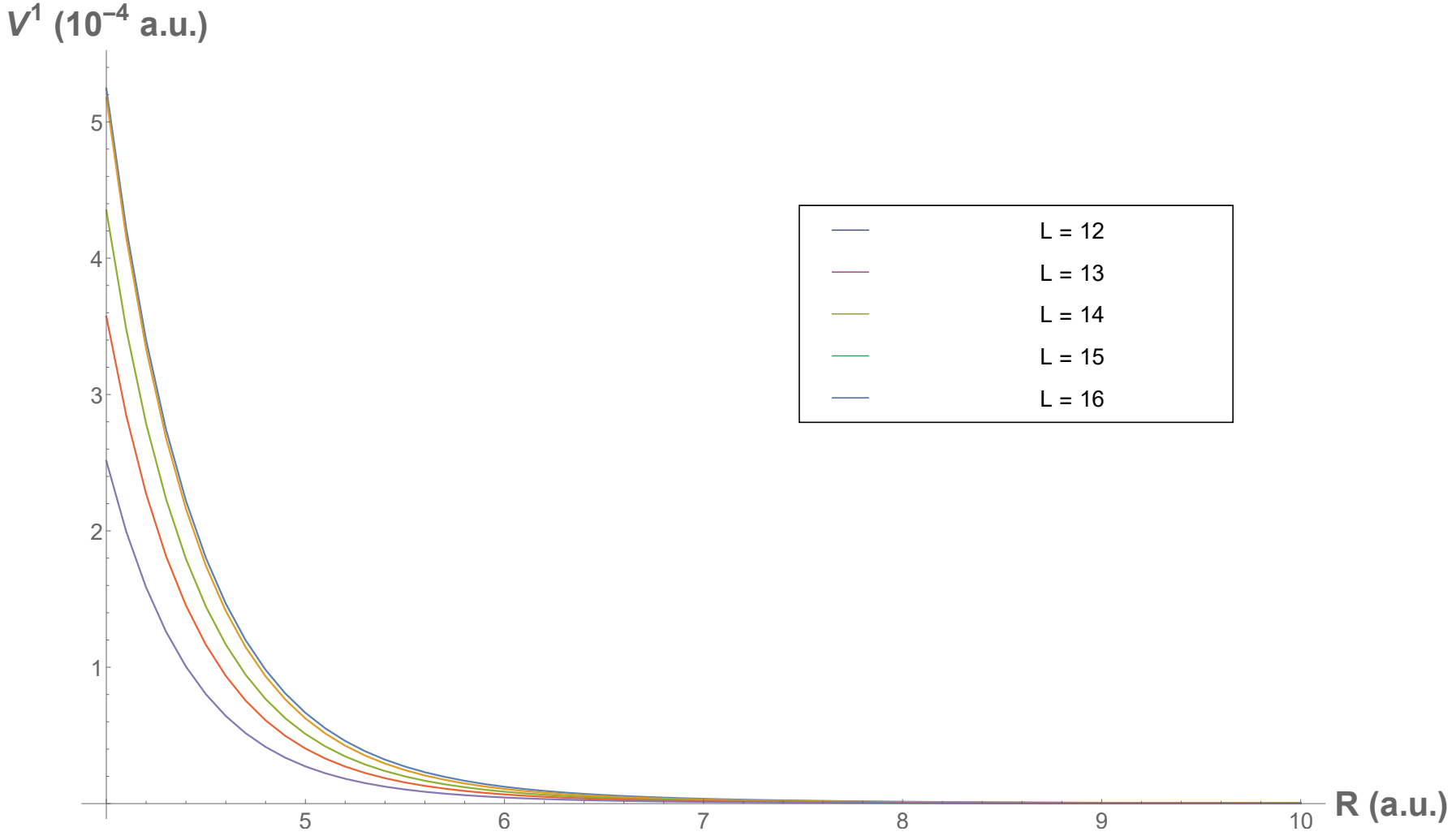
where

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

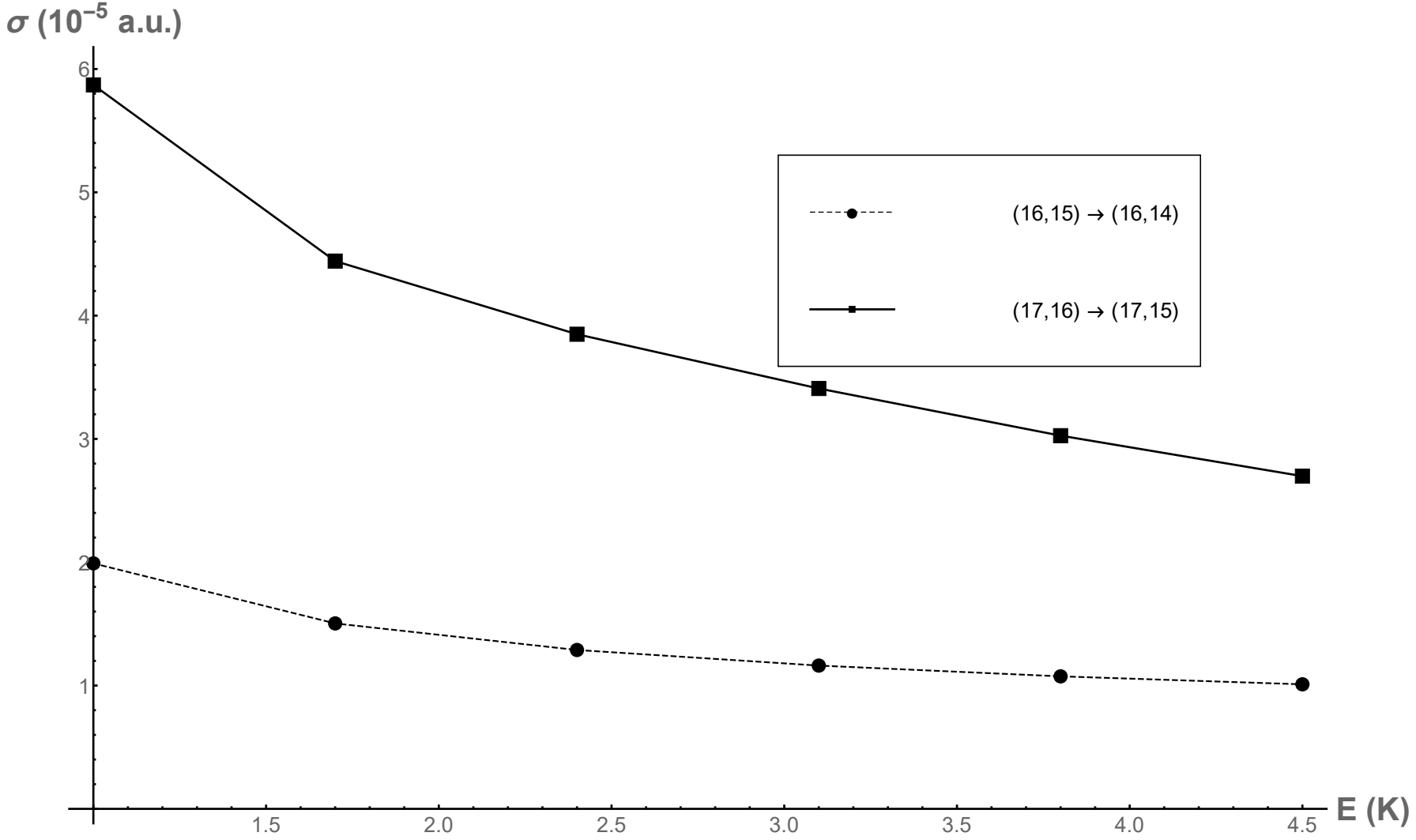
$$V^1_{nl,nl'}(R) = \int_0^\infty u_{nl}(r)u_{nl'}(r)V^1(r,R)r^2dr \quad (l' = l \pm 1)$$



Potentials $V^0_{nl}(R)$ for $n = 17$

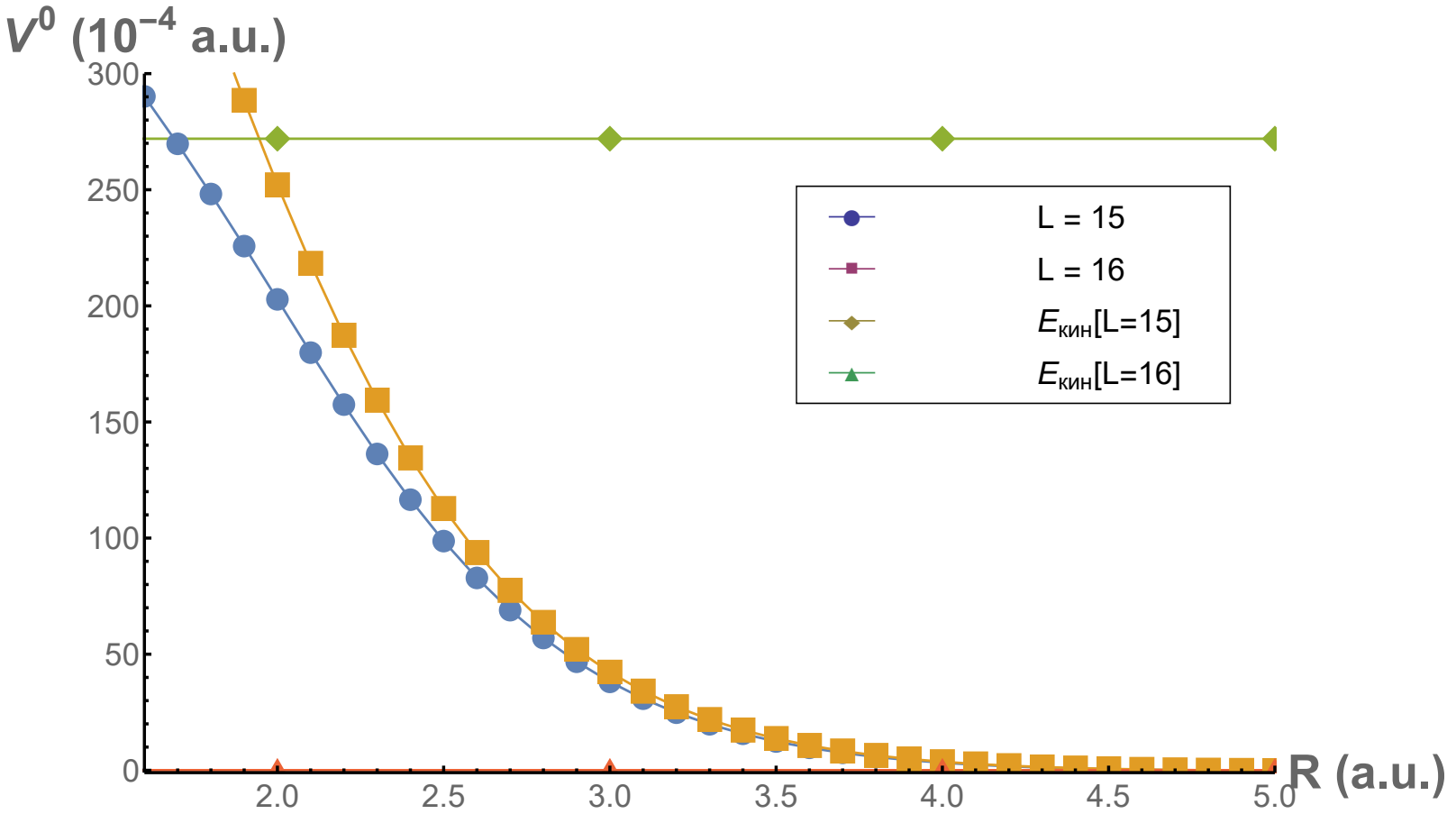


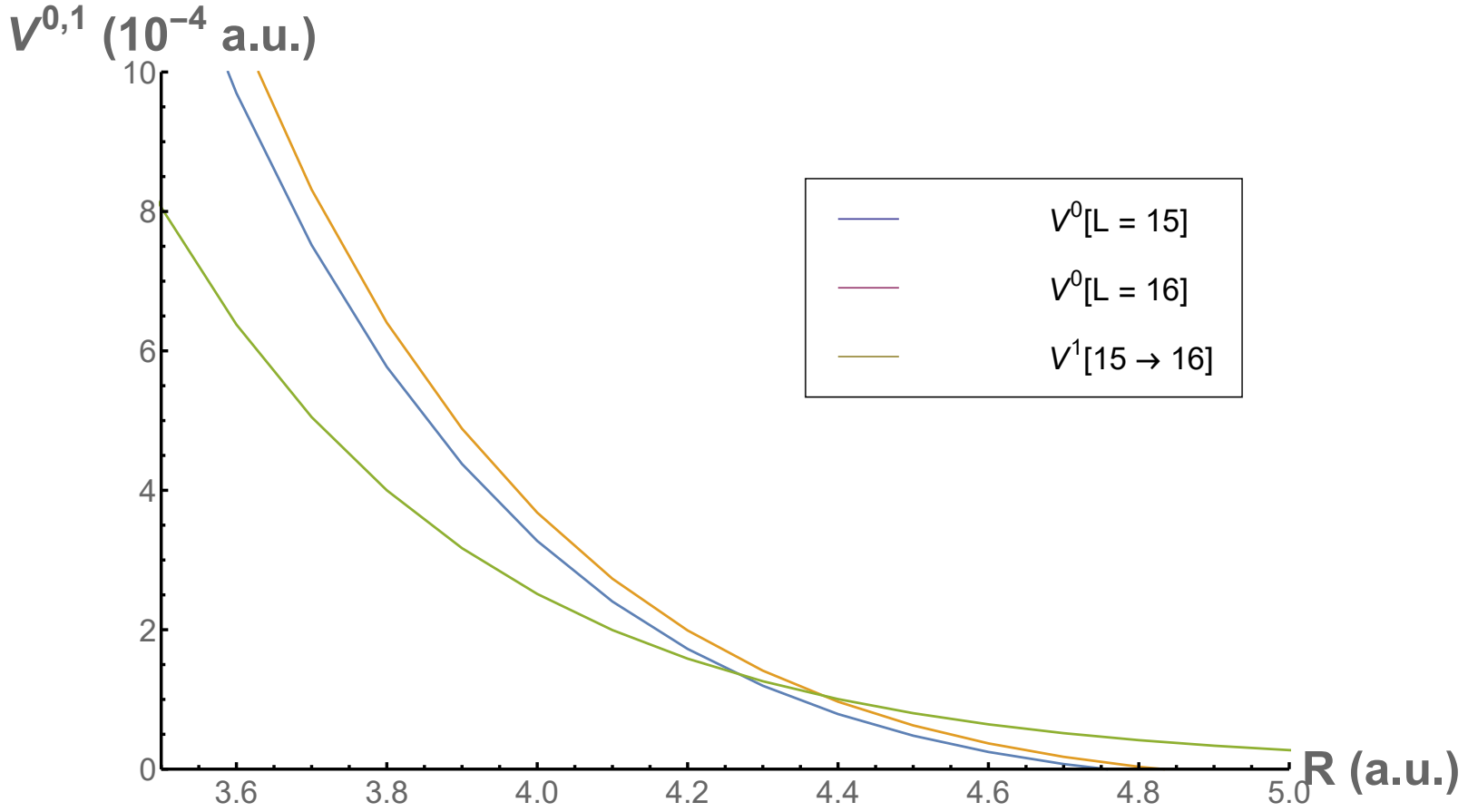
Potentials $V^1_{nl,nl-1}(R)$ for $n = 17$, $l = n - 1$



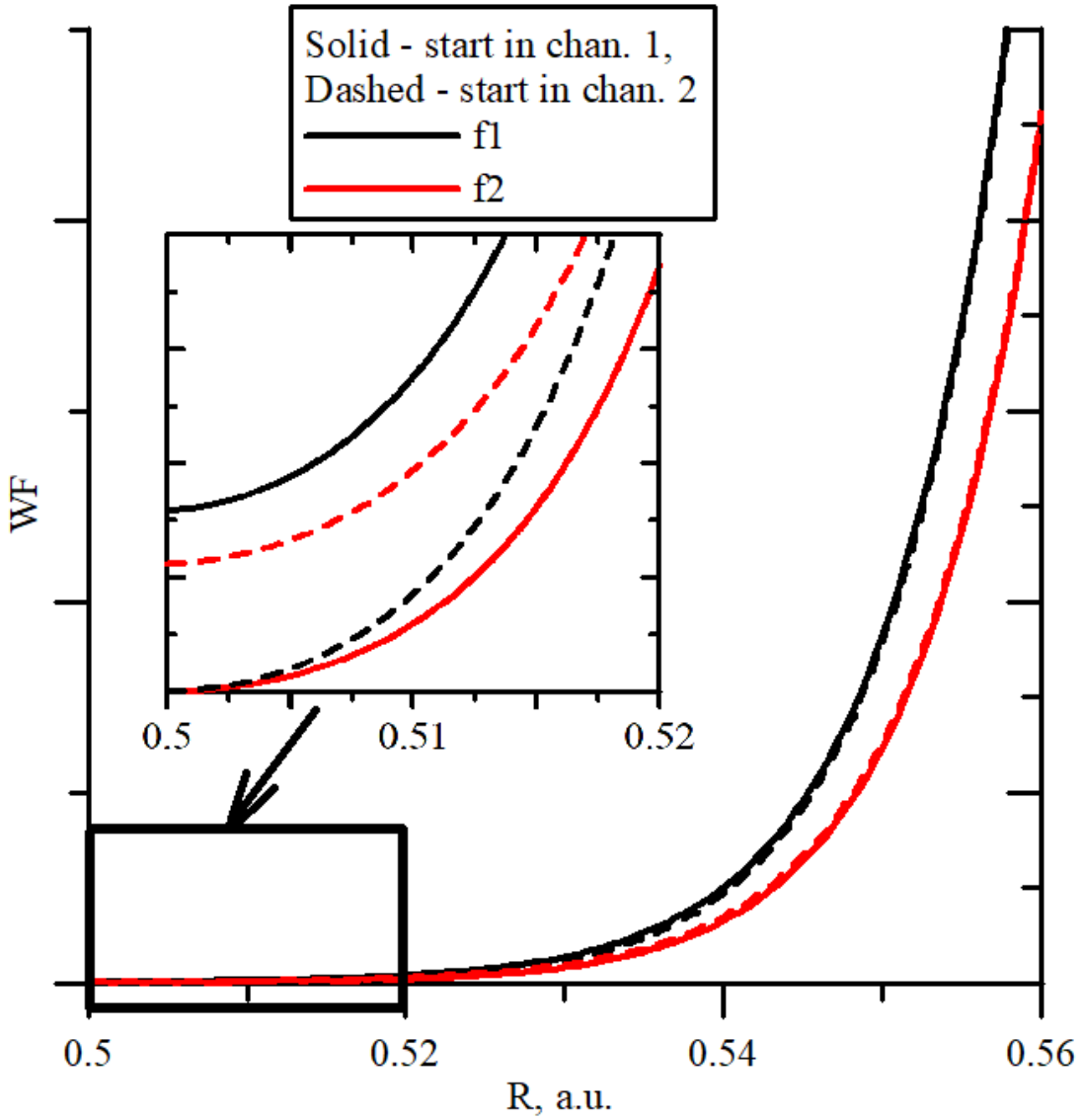
Cross sections of the transitions n, $l = n - 1 \rightarrow n\, l' = l - 1$

The cross section of the $(17, 16 \to 17, 15)$ transition is more than that one of the $(16, 15 \to 16, 14)$ transition by about 3 times.
Using the conversion constant $a_0^2 v_a = 6.126 \cdot 10^{-9}\,\mathrm{cm}^3/\mathrm{s}$ (from atomic to common units) and the density $\rho = 2.18 \cdot 10^{22}\,\mathrm{cm}^{-3}$ of a superfluid He at T=1.7 K we estimate a rate of collisional transition from the state (17,16) as $\lambda_{17,16} \simeq 3.2 \cdot 10^5\,\mathrm{s}^{-1}$, or lifetime with respect to quenching $\tau_q \simeq 3 \cdot 10^{-6}$ s.


V^0 (10^{-4} a.u.)
300
250
200
150
100
50
0
2.0
2.5
3.0
3.5
4.0
4.5
5.0
R (a.u.)
L = 15
L = 16
$E_{кин}$[L=15]
$E_{кин}$[L=16]


$V^{0,1}$ (10^{-4} a.u.)
10
8
6
4
2
0
3.6
3.8
4.0
4.2
4.4
4.6
4.8
5.0
R (a.u.)
V^0[L = 15]
V^0[L = 16]
V^1[15 → 16]

The solution forgot the initial value



Matrix degeneracy control of solutions at each step and orthogonalization (when necessary)

$(r_{min}, r_{max}) \to \{r_n\}$; i — channel number, α — boundary condition number, $y_i^{(\alpha)}$ — solution

$$\left|Y^{(\alpha)}\right\rangle = \begin{pmatrix} y_i^{(\alpha)} \\ y_i'^{(\alpha)} \end{pmatrix}$$ — vector of vawe function and its derivative

$$A = \left\langle Y^{(\alpha)} | Y^{(\beta)} \right\rangle = \sum_i \left[y_i^{(\alpha)} y_i^{(\beta)} + y_i'^{(\alpha)} y_i'^{(\beta)} / (k_i^2 + \delta_{reg}) \right]$$
— vector's scalar productions matrix

$$A \left|a^j\right\rangle = \lambda^j \left|a^j\right\rangle$$ — eigenvectors a^j with eigenvalues λ^j

$$\left|Y_{new}^{(\alpha)}(r_n)\right\rangle = \sum_j \left|a_j\right\rangle 1/\sqrt{\lambda^j} \left\langle a_j \middle| Y^{(\alpha)}(r_n)\right\rangle$$ — orthonormal vectors

Semi-analytical solution for stepped potential approximation

$$V_{ij}(r \in (r_i, r_{i+1})) = 2mV_{ij}^1(r_i) + \delta_{ij}\left[\frac{l(l+1)}{r_i^2} + 2m(V_i^0(r_i) - E_i)\right]$$

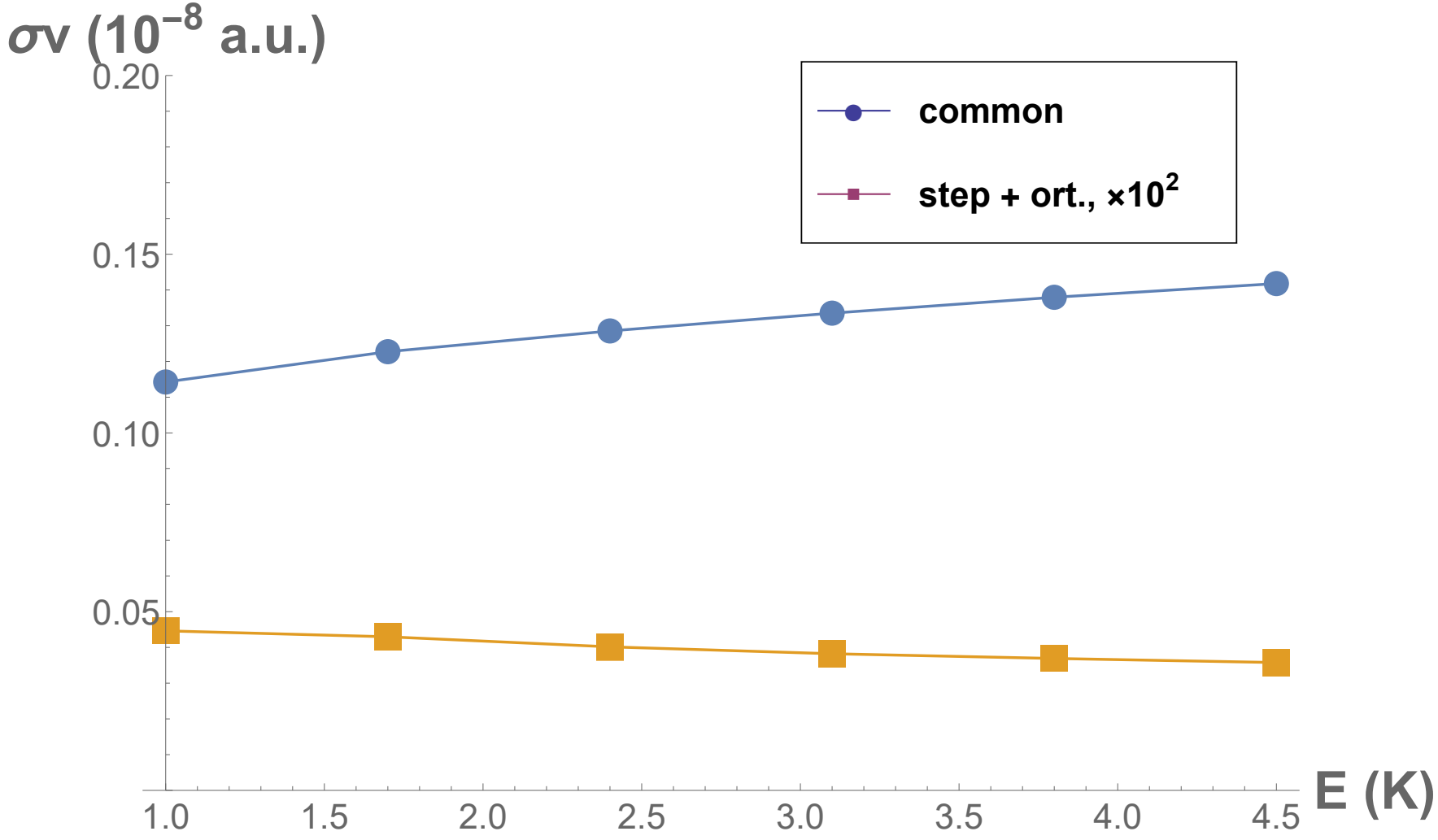
$\sum_j V_{ij} a_j^{(s)} = \lambda^{(s)} a_i^{(s)}$ — eigenvectors $a_j^{(s)}$ with eigenvalues $\lambda^{(s)}$

$$y_i'' = \sum_j V_{ij} y_j \quad \text{with} \quad y_i(r) = a_i^{(s)} f^{(s)}(r) \quad \text{lead to}$$

$$y_i''(r) = a_i^{(s)} f''^{(s)}(r) = \sum_j V_{ij} a_j^{(s)} f^{(s)}(r) = \lambda^{(s)} a_i^{(s)} f^{(s)}(r)$$

$$\Rightarrow f''^{(s)}(r) = \lambda^{(s)} f^{(s)}(r) \quad \text{is solved as}$$

$$f^{(s)}(r) = \begin{cases} A^{(s)} \sin[\sqrt{-\lambda^{(s)}} r] + B^{(s)} \cos[\sqrt{-\lambda^{(s)}} r] & \text{for } \lambda^{(s)} < 0 \\ A^{(s)} \exp[\sqrt{\lambda^{(s)}} r] + B^{(s)} \exp[-\sqrt{\lambda^{(s)}} r] & \text{for } \lambda^{(s)} > 0 \end{cases}$$



$\Gamma \approx 20\mathrm{GHz} \quad \Delta \approx 90\mathrm{GHz} \qquad \tau_q = 1/(n\sigma v) > 10^{-6}\mathrm{s}$