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Polarizability of the pionic helium atom

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Abstract

The static dipole polarizability of metastable states in pionic helium atoms is studied. We use the complex coordinate rotation method to properly take account of the resonant nature of the states. Our calculation shows that the (17, 14) states both in ³He and ⁴He are not stable due to strong collisional quenching. This explains the absence of signal in the PiHe experiment at the Paul Scherer Institute, Switzerland while studying the (16, 15) → (17, 14) transition.

Keywords: pionic mass, laser spectroscopy, dipole polarizability, complex coordinate rotation

1. Introduction

The pionic helium atom has attracted attention in recent years due to its potential to substantially improve precision in the determining the atomic mass of pion using laser spectroscopy [1]. In previous experiments the π^- mass was determined to a fractional precision of $(1-3) \times 10^{-6}$. These measurements were done mainly in two ways. First, by x-ray spectroscopy of exotic atoms πMg and πN , comparing the energies with relativistic bound-state calculations [2, 3]. The second way was measuring the recoil momentum of μ^+ [4] in the pion decay reaction: $\pi^+ \rightarrow \mu^+ \nu_\mu$, at rest.

The precision of the π^- mass determination using $\pi^- \text{He}^+$ will be ultimately limited by the natural width of the laser resonance determined by the lifetime $\tau_\pi \sim 26$ ns of π^- , compared to the transition energy ν_{exp} [1]. This implies that a fractional precision on the π^- mass of $< 10^{-8}$ can in principle be achieved, as in the case of the antiprotonic helium, $\bar{p}\text{He}^+$, [5]. In practice, systematic effects such as the shift and broadening of the resonance line due to atomic collisions and the collisional shortening of the state lifetimes can prevent the experiment from achieving this precision. One of the important characteristics that may provide us with some information for precision measuring of particular transitions is the electric dipole polarizability. There is another important issue, which will be seen from the calculated results presented in the final section: some states have very large polarizability and thus may become unstable under experimental conditions. Thus, these data help us to understand which states have regular behavior, and may give hints about a proper choice of transitions for precision laser spectroscopy.

The aim of this study is to perform comprehensive calculations regarding the polarizability properties of a set of metastable states of potential interest both for pionic ³He and ⁴He atoms. Atomic units are used throughout.

2. Theory

2.1. Wave function

The pionic helium atom consists of three interacting particles: π^- , the electron, and the helium nucleus. The strong interaction between π^- and the helium nucleus is strongly suppressed due to the centrifugal barrier (the angular momentum of a pionic orbital $l \approx 17$) and may be completely neglected.

The nonrelativistic Hamiltonian of a three-body system is taken in a form

$$H = -\frac{1}{2\mu_1} \nabla_{r_1}^2 - \frac{1}{2\mu_2} \nabla_{r_2}^2 - \frac{1}{M} \nabla_{r_1} \cdot \nabla_{r_2} - \frac{Z}{r_1} - \frac{Z}{r_2} + \frac{1}{r_{12}}, \quad (1)$$

where \mathbf{r}_1 and \mathbf{r}_2 are position vectors for two negative particles, $\mathbf{r}_{12} = \mathbf{r}_2 - \mathbf{r}_1$, $\mu_1 = Mm_1/(M + m_1)$ and $\mu_2 = Mm_2/(M + m_2)$ are reduced masses, M is a mass of helium nucleus, and $Z = 2$ is the nuclear charge. We assume that $m_1 = m_{\pi^-}$ and $m_2 = 1$, where m_{π^-} is a mass of a negative pion.

Pionic helium presents a quasi adiabatic system with a heavy pion orbiting over the helium nucleus with a velocity about 16 times slower than a remaining electron. On the other hand, it may be described as an atomic system with the

electron in its ground state: ψ_{1s} , with the pion occupying nearly circular orbital with principal and orbital quantum numbers, n and l . Due to interaction between the electron and pion, these quantum numbers are not exact and the wave function is determined by the total angular orbital momentum L and the excitation (or vibrational) quantum number ν , which are related to the atomic one as follows: $L = l, \nu = n - l - 1$.

In our calculations we use a variational expansion based on exponentials with randomly generated parameters. The wave functions are taken in the form

$$\Psi_L(l_1, l_2) = \sum_{k=1}^{\infty} \left\{ U_k \operatorname{Re} \left[e^{-\alpha_k r_1 - \beta_k r_2 - \gamma_k r_{12}} \right] + W_k \operatorname{Im} \left[e^{-\alpha_k r_1 - \beta_k r_2 - \gamma_k r_{12}} \right] \right\} \mathcal{Y}_{LM}^{l_1 l_2}(\mathbf{r}_1, \mathbf{r}_2), \quad (2)$$

where $\mathcal{Y}_{LM}^{l_1 l_2}(\mathbf{r}_1, \mathbf{r}_2)$ are the solid bipolar harmonics as defined in [6],

$$\mathcal{Y}_{LM}^{l_1 l_2}(\mathbf{r}_1, \mathbf{r}_2) = r_1^{l_1} r_2^{l_2} \{ Y_{l_1} \otimes Y_{l_2} \}_{LM},$$

and L is the total orbital angular momentum of a state. Complex parameters α_k, β_k , and γ_k are generated in a quasirandom manner [7, 8]:

$$\alpha_k = \left[\left[\frac{1}{2} k(k+1) \sqrt{p_\alpha} \right] (A_2 - A_1) + A_1 \right] + i \left[\left[\frac{1}{2} k(k+1) \sqrt{q_\alpha} \right] (A_2' - A_1') + A_1' \right], \quad (3)$$

where $[x]$ designates the fractional part of x , p_α and q_α are some prime numbers, and $[A_1, A_2]$ and $[A_1', A_2']$ are real variational intervals, which need to be optimized. Parameters β_k and γ_k are obtained in a similar way.

More details may be found in [9].

2.2. The complex coordinate rotation method and perturbation theory

The Coulomb Hamiltonian (1) is analytic under dilatation transformations

$$(U(\theta)f)(\mathbf{r}) = e^{m\theta/2} f(e^\theta \mathbf{r}), \quad H(\theta) = U(\theta) H U^{-1}(\theta), \quad (4)$$

for real θ , or in other words it may be expanded in a convergent power series of the dilatation parameter θ on some open interval, and thus can be analytically continued to the complex plane. Parameter m in equation (4) is a dimension of the coordinate space, say, for a single electron in a three-dimensional space: $m = 3$.

The complex coordinate rotation (CCR) method [10] ‘rotates’ the coordinates of the dynamical system ($\theta = i\varphi$), $r_{ij} \rightarrow r_{ij} e^{i\varphi}$, where φ is the parameter of the complex rotation. Under this transformation the Hamiltonian (1) changes as a function of φ

$$H_\varphi = T e^{-2i\varphi} + V e^{-i\varphi}, \quad (5)$$

where T and V are the kinetic energy and Coulomb potential operators. The continuum spectrum of H_φ is rotated on the

complex plane around branch points (‘thresholds’) to ‘uncover’ resonant poles situated on the unphysical sheet of the Riemann surface in accordance with the Augilar–Balslev–Combes theorem [11]. The resonance energy is then determined by solving the complex eigenvalue problem for the ‘rotated’ Hamiltonian

$$(H_\varphi - E)\Psi_\varphi = 0. \quad (6)$$

The eigenfunction Ψ_φ obtained from equation (6) is square-integrable, and the corresponding complex eigenvalue $E = E_r - i\Gamma/2$ defines the energy E_r and the width of the resonance, Γ , the latter being related to the Auger rate as $\lambda_A = \Gamma/\hbar$.

The use of a finite set of N basis functions defined by (2) reduces the problem (6) to the generalized algebraic complex eigenvalue problem

$$(A - \lambda B)x = 0, \quad (7)$$

where $A = \langle \Psi_\varphi | H_\varphi | \Psi_\varphi \rangle$ is the finite $N \times N$ matrix of the Hamiltonian in this basis, and B is the matrix of overlap $B = \langle \Psi_\varphi | \Psi_\varphi \rangle$.

To evaluate the static dipole polarizability for the CCR states, a second-order perturbation theory is required. The relevant background is provided by the theorem [12].

Theorem. *Let H be a three-body Hamiltonian with Coulomb pairwise interaction, and $W(\theta)$ be a dilatation analytic ‘small’ perturbation of a complex parameter θ (in the CCR case, $\theta = i\varphi$, where φ is a rotational angle). Let E_0 be an isolated simple resonance energy (discrete eigenvalue of $H(\theta)$). Then for β small, there is exactly one eigenstate of $H(\theta) + \beta W(\theta)$ near E_0 and*

$$E(\beta) = E_0 + a_1 \beta + a_2 \beta^2 + \dots \quad (8)$$

is analytic near $\beta = 0$. In particular,

$$a_1 = E'(0) = \langle \Psi_0^*(\theta) | W(\theta) | \Psi_0(\theta) \rangle, \quad a_2 = \sum_{n \neq 0} \frac{\langle \Psi_0^*(\theta) | W(\theta) | \Psi_n(\theta) \rangle \langle \Psi_n^*(\theta) | W(\theta) | \Psi_0(\theta) \rangle}{E_0 - E_n(\theta)}, \quad (9)$$

where the sum is carried out over the states of discrete and continuum spectra of the rotated Hamiltonian $H(\theta)$ (in case of numerical solution the summation over all pseudostates is performed).

It is assumed that the wave functions are normalized as $\langle \Psi^*(\theta), \Psi(\theta) \rangle = 1$. Coefficients a_1, a_2 , etc do not depend on θ , if only rotated branches of the continuum spectrum of $H(\theta)$ uncover E_0 and its vicinity on the complex plane. These coefficients are complex and the imaginary part contributes to the width of the resonance as it follows from equation (8).

2.3. Polarizabilities

The interaction with an external electric field in the dipole interaction form is expressed by

$$V_p = -\mathcal{E} \cdot \mathbf{d}, \quad \mathbf{d} = e(Z \mathbf{R}_N - \mathbf{R}_{\pi^-} - \mathbf{R}_e) \quad (10)$$

where \mathbf{d} is the electric dipole moment of the three particles with respect to the center of mass of the system. It is easy to check that the perturbation operator is dilatation analytic and transforms with rotation parameter φ as (cf equation (5)) $\mathbf{d}_\varphi = \mathbf{d} e^{i\varphi}$.

The change of energy due to polarizability of molecular ions is expressed by

$$\begin{aligned} E_p^{(2)} &= \langle \Psi_0 | V_p (E_0 - H_0)^{-1} V_p | \Psi_0 \rangle \\ &= E^i E^j \langle \Psi_0 | d^i (E_0 - H_0)^{-1} d^j | \Psi_0 \rangle = -\frac{1}{2} \alpha_d^{ij} \mathcal{E}^i \mathcal{E}^j, \end{aligned} \quad (11)$$

where α^{ij} is a tensor of polarizability of rank 2,

$$\alpha_d^{ij} = -2 \langle \Psi_0 | d^i (E_0 - H_0)^{-1} d^j | \Psi_0 \rangle. \quad (12)$$

The static dipole polarizability tensor is then reduced [13] to scalar, α_s , and tensor, α_t , terms, which may be expressed in terms of three contributions (we follow notation of [14]) corresponding to the possible values of L' for the angular momentum of the intermediate state: $L' = L \pm 1$, or $L' = L$.

$$\begin{aligned} a_+ &= \frac{2}{2L+1} \sum_n \frac{\langle 0L || \mathbf{d} || n(L+1) \rangle \langle n(L+1) || \mathbf{d} || 0L \rangle}{E_0 - E_n}, \\ a_0 &= -\frac{2}{2L+1} \sum_n \frac{\langle 0L || \mathbf{d} || nL \rangle \langle nL || \mathbf{d} || 0L \rangle}{E_0 - E_n}, \\ a_- &= \frac{2}{2L+1} \sum_n \frac{\langle 0L || \mathbf{d} || n(L-1) \rangle \langle n(L-1) || \mathbf{d} || 0L \rangle}{E_0 - E_n}. \end{aligned} \quad (13)$$

Here, E_n is the energy of the intermediate state $|nL'\rangle$. The polarizability tensor operator on a subspace of fixed total orbital angular momentum L may now be expressed:

$$\alpha_d^{ij} = \alpha_s + \alpha_t \left[L^i L^j + L^j L^i - \frac{2}{3} \mathbf{I}^2 \right], \quad (14)$$

where

$$\begin{aligned} \alpha_s &= \frac{1}{3} [a_+ + a_0 + a_-], \\ \alpha_t &= -\frac{a_+}{2(L+1)(2L+3)} \\ &\quad + \frac{a_0}{2L(L+1)} - \frac{a_-}{2L(2L-1)}. \end{aligned} \quad (15)$$

Numerical calculation of the latter two quantities, α_s and α_t , is the main objective of the present work. In general, these coefficients are complex numbers and the imaginary part may be interpreted as a contribution to the Auger width of a particular M substate (see equation (8)).

Table 1. Test of convergence of scalar α_s and tensor α_t polarizability calculations for the states of the ${}^4\text{He}^+\pi^-$ atom. N' is the number of intermediate states for each angular momentum subspace: $L' = L, L \pm 1$.

state	N'	α_s	$\alpha_t \times 10^3$
(16, 15)	1200	0.61671 + <i>i</i> 0.00503	2.0152 - <i>i</i> 0.01734
	1600	0.61662 + <i>i</i> 0.00496	2.0155 - <i>i</i> 0.01711
	2000	0.61665 + <i>i</i> 0.00496	2.0154 - <i>i</i> 0.01711
(17, 14)	1600	35219. + <i>i</i> 1289.	-54888. - <i>i</i> 6329.
	2000	38504. + <i>i</i> 1446.	-65007. - <i>i</i> 4333.
	2500	40211. + <i>i</i> 1310.	-69854. - <i>i</i> 3537.
	3000	40802. + <i>i</i> 1240.	-72055. - <i>i</i> 3720.

3. Results and discussion

In our calculations the initial states were obtained using variational expansion (2) by the CCR method. Basis sets up to $N = 2000$ had been used to get the complex energy of a state with a relative precision of 10^{-10} - 10^{-14} , which depends primarily on the Auger width of a state. Intermediate states were obtained using the same variational expansion for substates of angular momentum $L' = L, L \pm 1$. A number of basis functions for intermediate states was taken to be of the same size as for an initial state, namely, $N' = 2000$ for each substate L' of angular momentum. In some complicated cases of ‘anomalous’ states (see below), a number of basis functions taken increased up to $N = 3000$. The states are labeled by two numbers (n, l), the principal quantum number n and orbital momentum l of the pionic orbital as is explained in section 2.1.

Convergence of the polarizability coefficients, α_s and α_t , as they are defined by equations (14) and (15), was also studied. Results of convergence tests for the ‘regular’ (16, 15) state and the ‘anomalous’ (17, 14) state are presented in table 1. As is seen from the table, in the latter case the state has very large polarizability and much poor convergence. Such anomalous behavior may be explained by strong correlation with the excited electron ‘Rydberg’ states, which occur in close vicinity to the initial state on the Riemann surface of complex energy. These excited states have much broader Auger width, and such closeness begins to affect the polarizability and stability of the initial atomic state. In the case of the antiprotonic helium, such states were discussed in [15]. It was observed in experiment [16] that in dense targets these states have a much shorter lifetime than it is predicted by the calculated Auger lifetime within the assumption of an isolated atom.

Final results are presented in tables 2 and 3. For comparison, polarizability of the ground state in the helium atom is $\alpha_s = 1.383\dots$ In these tables, printed digits of the polarizability coefficients are all significant. With few exceptions, proper convergence has not been achieved either in the (17, 14) state in the ${}^3\text{He}$ and ${}^4\text{He}$ atoms or in the (17, 15) state in the ${}^3\text{He}$ atom. It is clearly seen that in the case of ‘regular’ states (with a small imaginary part in polarizability) the tensor polarizability grows rapidly with an increase in the principal quantum number n of the pionic orbital. It means that the geometry of the states becomes less and less spherically

Table 2. Nonrelativistic energies E_{nr} (in a.u.), Auger widths Γ (in a.u.), scalar α_s and tensor α_t polarizabilities for the ${}^4\text{He}^+\pi^-$ atom.

state	E_{nr}	$\Gamma/2$	α_s	$\alpha_t \times 10^3$
(15, 14)	-3.0569481417(4)	$5.14 \cdot 10^{-6}$	$1.0319 + i0.0575$	$1.9299 - i0.2280$
(16, 14)	-2.858617029(2)	$4.83 \cdot 10^{-5}$	$5.4240 + i0.4408$	$-9.2097 - i1.5058$
(16, 15)	-2.82854939373(4)	$2.1 \cdot 10^{-10}$	$0.6166 + i0.0049$	$2.0155 - i0.0171$
(17, 14)	-2.70984178(2)	$2.00 \cdot 10^{-6}$	$40802. + i1240.0$	$-72055. - i3720.2$
(17, 15)	-2.68542722(2)	$2.50 \cdot 10^{-6}$	$0.5520 + i1.8844$	$-3.3536 + i7.0089$
(17, 16)	-2.65751243850171	$1.0 \cdot 10^{-13}$	$-0.1033 + i0.0002$	$3.3333 - i0.0006$
(18, 15)	-2.58002554(1)	$6.53 \cdot 10^{-6}$	$-0.5937 + i0.1075$	$8.6596 - i0.3070$
(18, 16)	-2.556984919572(2)	$1.3 \cdot 10^{-11}$	$-0.2987 + i0.0018$	$5.1904 - i0.0053$
(18, 17)	-2.5319465695913	—	-0.9661	5.1114
(19, 15)	-2.50049819(2)	$2.55 \cdot 10^{-5}$	$1.9255 + i0.6604$	$7.0935 - i2.0690$
(19, 16)	-2.481540552377(5)	$1.95 \cdot 10^{-10}$	$-0.2737 + i0.0500$	$8.4719 - i0.1512$
(19, 17)	-2.4618067856861	—	-1.1987	8.2456
(19, 18)	-2.4413857971745	—	-2.4015	8.4059

Table 3. Nonrelativistic energies E_{nr} (in a.u.), Auger widths Γ (in a.u.), scalar α_s and tensor α_t polarizabilities for the ${}^3\text{He}^+\pi^-$ atom.

state	E_{nr}	$\Gamma/2$	α_s	$\alpha_t \times 10^3$
(15, 14)	-3.0342533945(3)	$5.53 \cdot 10^{-6}$	$0.9873 + i0.0531$	$2.0164 - i0.1938$
(16, 14)	-2.840170981(2)	$3.79 \cdot 10^{-5}$	$2.5933 + i0.2178$	$-1.1745 - i0.7453$
(16, 15)	-2.81027798905(1)	$3.47 \cdot 10^{-10}$	$0.5278 + i0.0027$	$2.2422 - i0.0094$
(17, 14)	-2.695209116(1)	$4.34 \cdot 10^{-7}$	$2175.2 + i33.447$	$-3215.1 - i92.822$
(17, 15)	-2.6709980910(1)	$6.0 \cdot 10^{-9}$	$664.40 + i11.180$	$-945.32 - i32.859$
(17, 16)	-2.643122610302	$2.0 \cdot 10^{-12}$	$-0.1744 + i0.0002$	$3.5105 - i0.0006$
(18, 15)	-2.568490191(5)	$5.84 \cdot 10^{-6}$	$-0.6687 + i0.1356$	$9.0307 - i0.5149$
(18, 16)	-2.545645472099	$3.3 \cdot 10^{-11}$	$-0.3534 + i0.0016$	$5.4609 - i0.0049$
(18, 17)	-2.52088142679	—	-1.0790	5.4315
(19, 15)	-2.49096242(3)	$1.55 \cdot 10^{-5}$	$-0.5020 + i0.4120$	$14.391 - i0.9111$
(19, 16)	-2.47237023589	$2.2 \cdot 10^{-10}$	$-0.5433 + i0.0181$	$9.6460 - i0.0548$
(19, 17)	-2.452935974501	—	-1.2556	8.6402
(19, 18)	-2.432980844931	—	-2.6204	9.0244

symmetric, which should in turn increase the Stark quenching of the high n states.

A natural question arises: is the second-order perturbation still applicable in the case of huge polarizability of a state? In order to answer this question we may evaluate approximate second-order perturbation energy for the (17, 14) state in the ${}^4\text{He}$ pionic atom under experimental conditions. The largest electric field appears in collisions of the pionic helium with surrounding atoms. The mean distance in the liquid helium target is about 10 Bohr radii and results in the electric field strength, which gives the energy shift $\Delta E_p^{(2)} \approx 10^{-9}$ a.u. As is seen from table 2, that is three orders of magnitude less than the natural width of this state. Still, that may change the wave function configuration, which should acquire some admixture of the excited electron Rydberg state lying in the vicinity. At a distance of 5 Bohr radii the strength of the electric field becomes too large and we may expect realignment of the wave function and the immediate disappearance of the state due to emission of an Auger electron.

In the Paul Scherer Institute (PSI) experiment the first attempt to find a signal was by inducing the (16, 15) \rightarrow (17,

14) transition in ${}^4\text{He}^+\pi^-$ [17] by a laser pulse irradiation. We have tried to explain above why this attempt was unsuccessful. The other example of a doubtful state for spectroscopic studies is the (17, 15) state in $\pi^3\text{He}$.

According to the theory, which allows us to evaluate the initial population of the metastable states [18, 19], and which has been developed for antiprotonic helium and previously confirmed by experiment [20], the main hypothesis related to the pionic helium case is that initially the most populated state should be the (16, 15) state and its life time due to collisional quenching under the conditions of the present experiment at PSI is 7 ns. Thus it is appealing but challenging to try to induce the (16, 15) \rightarrow (17, 16) transition, which in the case of an expectedly different quenching rate for the upper state may cause visible changes in the observed time spectrum of the pion absorption.

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