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LETTER TO THE EDITOR

The search for oscillations in the near-threshold photo-double ionization cross section of helium

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Abstract

The photo-double ionization cross section for the helium atom is calculated in the near-threshold region by direct solution of the time-dependent Schrödinger equation. Full close-coupling results for the $1s^2\ ^1S$ ground state are found to be in excellent agreement with experimental measurements. The calculations confirm the validity of the Wannier power law from 0.1 eV to about 1.7 eV excess energy and find no oscillations in the threshold cross section beyond numerical uncertainty. Further time-dependent calculations are made in a simpler *s*-wave counterlinear model for both the $1s^2\ ^1S$ ground and $1s2s\ ^1S$ excited states. Although numerical uncertainties are significantly reduced in the helium model calculations, again no oscillations in the threshold cross sections are found beyond the remaining numerical uncertainty.

A classic example of the quantal three-body Coulomb problem is the photo-double ionization of an atom. The emission of two electrons following the absorption of just one photon by a target atom cannot occur in the absence of electron–electron correlations due to the single-particle nature of the dipole interaction. The near-threshold region for the escape of two electrons is a particularly challenging problem for *ab initio* theory since both electrons move slowly and interact with each other for quite a long time, thus invalidating the use of low-order quantal perturbation theory.

Two different semi-empirical theories have been developed which model the energy dependence of the photo-double ionization cross section near threshold. An early classical dynamics analysis, carried out by Wannier [1], derived a power law dependence for the near-threshold electron-impact ionization cross section of hydrogen. For the photo-double ionization of ground-state helium, the cross section is given by

$$\sigma^{2+} = \sigma_0 E_{\rm exc}^{\alpha}, \tag{1}$$

where $E_{\rm exc}$ is the excess energy and the Wannier exponent α equals 1.056. The classical picture is that by the time the two electrons are ejected they are approximately at the same

distance from the nucleus and have almost identical kinetic energies, but move in opposite directions. The semi-classical theories of Rau [2] and Peterkop [3] and the higher-order theory of Feagin [4] show how this threshold law could be obtained from a quantum treatment. In fact, there is an extensive set of treatments by many different authors that obtain the threshold law and corrections to it. In particular an oscillating, but still monotonically increasing cross section near threshold has been derived by Temkin and Hahn [5] originally for electron-impact ionization of atoms and photo-double detachment of negative ions. It is based on the picture that one of the two electrons leaves the atom much faster than the other one does and thus is governed by a dipole field and not by a Coulomb field as the system of residual ion and slower leaving electron is essentially neutral. Recently, Temkin and Hahn's theory has been extended to photo-double ionization of atoms (see [6, 7] and references therein) and accounts for an additional Coulomb field which is seen by the faster leaving electron as, in this case, the residual ion is doubly and not singly charged.

The pioneering experiment by Kossmann *et al* [8] mapped out the photo-double ionization of helium in great detail between about 0.17 eV and 4.0 eV excess energy. A power law dependence of the cross section was observed in agreement with the Wannier theory, but no oscillations were seen. Recently, however, experimental studies of the photo-double ionization of lithium [6] and beryllium [7] near threshold have reported oscillatory structures in these cross sections outside experimental uncertainties. Although the magnitude of the oscillations may be different due to the varying atomic structure of the atoms studied, it may be argued that the presence or absence of oscillations should be a universal feature in the near-threshold region of any atom.

In the last decade, a number of *ab initio* non-perturbative quantal methods have been applied to calculate the photo-double ionization of light atoms. The photo-double ionization of ground-state helium has been calculated using the convergent close-coupling [9–13], time-dependent close-coupling [14–16], hyperspherical R-matrix [17–19], B-spline based R-matrix [20], and exterior complex scaling [21] methods, while the photo-double ionization of the lowest-excited states of helium have been calculated using the convergent close-coupling [22], time-dependent close-coupling [23], and B-spline based R-matrix [20, 24] methods. The convergent close-coupling [25], time-dependent close-coupling [26], and hyperspherical R-matrix [27] methods have also been applied to the photo-double ionization of the outer subshell electrons of ground-state beryllium. Recently, the time-dependent close-coupling method has been employed to calculate the photo-double and photo-triple ionization cross sections for both lithium [28, 29] and beryllium [29]. All of these advanced *ab initio* non-perturbative methods are computationally intensive and become increasingly difficult to converge at the small excess energies found in the near-threshold region. For example, the convergent close-coupling results for the photo-double ionization of the ground state [11] and the lowest-excited states [22] of helium do not extend below 1.0 eV excess energy due to limited computational resources.

In this letter, we apply the time-dependent close-coupling method to calculate the photo-double ionization cross section for ground-state helium between 0.1 eV and 2.5 eV excess energy. Our absolute cross sections are then compared to semi-empirical threshold law predictions, as well as experimental measurements [8]. Further time-dependent calculations are made in a simpler s-wave counterlinear model for both the $1s^2\ ^1S$ ground and $1s2s\ ^1S$ excited states of helium. As expected, the numerical uncertainties in the model calculations are found to be significantly reduced when compared to the full close-coupling calculations. Our model cross sections are then examined near threshold in a further search for oscillations. Atomic units are used unless stated otherwise.

In the time-dependent close-coupling method, the wavefunction for ground-state helium exposed to dipole radiation may be separated as

$$\Psi_{\text{total}}(\vec{r}_1, \vec{r}_2, t) = \Phi_0^{^1\text{S}}(\vec{r}_1, \vec{r}_2)\, \mathrm{e}^{-\mathrm{i}E_0 t} + \Psi^{^1\text{P}}(\vec{r}_1, \vec{r}_2, t) \tag{2}$$

where $\vec{r}_1$ and $\vec{r}_2$ denote the two electron coordinates and, at time $t = 0$, the second term is set to zero. The wavefunction $\Phi_0^{^1\text{S}}$ for the ground state of helium is obtained by relaxation of a trial function fulfilling the Schrödinger equation

$$-\frac{\partial \Phi_0^{^1\text{S}}(\vec{r}_1, \vec{r}_2, \tau)}{\partial \tau} = H_{\text{atom}} \Phi_0^{^1\text{S}}(\vec{r}_1, \vec{r}_2, \tau) \tag{3}$$

in imaginary time ($\tau = \mathrm{i}t$). The non-relativistic Hamiltonian for helium with its nucleus of charge $Z = 2$ at rest at the origin of the coordinate system reads

$$H_{\text{atom}} = -\frac{1}{2}\Delta_1 - \frac{Z}{r_1} - \frac{1}{2}\Delta_2 - \frac{Z}{r_2} + \frac{1}{|\vec{r}_1 - \vec{r}_2|}. \tag{4}$$

If one-photon absorption is the only relevant process (weak-field perturbative limit), then the wavefunction (2) satisfies the following time-dependent Schrödinger equation

$$\mathrm{i}\frac{\partial \Psi^{^1\text{P}}(\vec{r}_1, \vec{r}_2, t)}{\partial t} = H_{\text{atom}} \Psi^{^1\text{P}}(\vec{r}_1, \vec{r}_2, t) + H_{\text{field}} \Phi_0^{^1\text{S}}(\vec{r}_1, \vec{r}_2)\, \mathrm{e}^{-\mathrm{i}E_0 t}. \tag{5}$$

In the length gauge, the Hamiltonian of a classical time-dependent electric field fully linearly polarized along the z axis may be written as

$$H_{\text{field}} = E(t)(r_1 \cos\theta_1 + r_2 \cos\theta_2) \sin(\omega t) \tag{6}$$

with $E(t)$ being the time-dependent amplitude and ω the frequency. The velocity gauge may also be used, but previous calculations on helium [14, 23] have been found to be gauge invariant. The amplitude has to be ramped on slowly to avoid ringing effects. In the present time-dependent close-coupling calculation, the amplitude is ramped on as follows:

$$\begin{aligned} E(t) &= 4t/t_{\text{tot}} \qquad \text{for} \quad t < t_{\text{tot}}/4 \\ E(t) &= 1 \qquad\qquad\ \ \text{for} \quad t \geqslant t_{\text{tot}}/4 \end{aligned} \tag{7}$$

where t_{tot} is the total time equation (5) has to be time-propagated to obtain converged cross sections. The propagation time t_{tot} has to be longer for smaller excess energies.

For the numerical solution of the time-dependent Schrödinger equation (5), the wavefunctions $\Phi_0^{^1\text{S}}$ and $\Psi^{^1\text{P}}$ are expanded in two-electron coupled spherical harmonics with orbital angular momenta up to 2 for the former and up to 3 for the latter, respectively. For details see [14, 30]. By this, equation (5) is transformed into a set of coupled partial differential equations for two-electron radial wavefunctions. This set is solved on a non-uniform lattice consisting of 2784 × 2784 points. The initial mesh spacing of $\Delta r_{\text{min}} = 0.1$ au is increased by 0.0005 au at each mesh point up to a final mesh spacing of $\Delta r_{\text{max}} = 0.4$ au and held constant afterwards. This yields a huge lattice of size 1023.45 au × 1023.45 au which allows us to time-propagate equation (5) long enough to converge the photo-double ionization cross section at small excess energies. As described in [14, 30] projection techniques are used to obtain cross sections from the time-evolved two-electron radial wavefunctions. Projection is done onto a complete set of one-electron bound states. This is an excellent approximation, as fully evolved in time, the interaction of the two electrons becomes quite small in regard to their kinetic energies. Since this approximation becomes more accurate as the lattice size increases convergence checks of the photo-double ionization cross section versus the lattice size can be made. The radial parts of the bound one-electron wavefunctions are obtained by diagonalizing the time-independent radial Hamiltonian of He^+ on a one-dimensional lattice

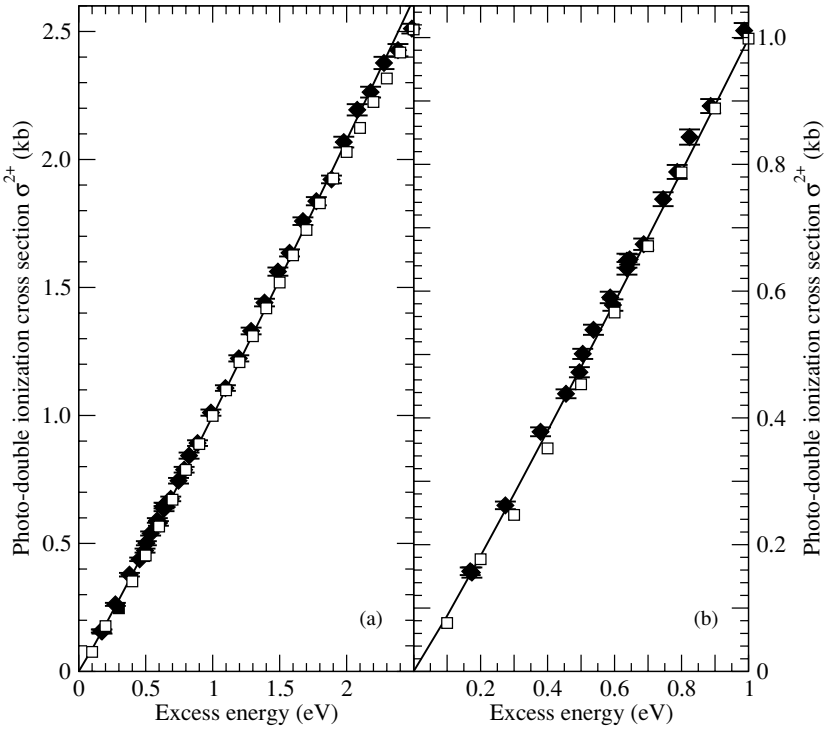

Figure 1. Cross section for photo-double ionization of ground-state helium as a function of the excess energy plotted for two different energy ranges: □ TDCC data, ♦ experimental data due to Kossmann *et al* [8], —— Wannier power law (1) with the TDCC proportionality constant $\sigma_0 = 0.998$ kb.

which has the same number of points and the same non-uniform mesh spacing as that used for the two-electron system.

Figure 1(a) displays our time-dependent close-coupling (TDCC) cross section for photo-double ionization of ground-state helium as a function of the excess energy up to 2.5 eV, while figure 1(b) gives an enlarged view of the same cross section for excess energies up to 1.0 eV only. The solid line represents the Wannier power law (1) with $\alpha = 1.056$ and the TDCC value for the proportionality constant, which is $\sigma_0 = 0.998$ kb. This is our cross section at 1.0 eV excess energy. We have not done any least-squares fits to our TDCC data as the low-energy points, where the threshold law will hold most accurately, are the least well known in our calculation. Using these values, it is evident from figure 1(a) that the cross section starts to deviate from the Wannier power law at about 1.7 eV excess energy. At higher excess energies, the cross section becomes visibly smaller than the one that the Wannier power law predicts. Almost at threshold, i.e. for excess energies up to about 0.5 eV, our TDCC cross section lies below the Wannier curve and, thus, may not be fully converged. In the near-threshold region, the cross section for photo-double ionization converges extremely slowly. While the Schrödinger equation (5) had to be time propagated over just 10–15 electric field periods at moderate excess energies [16], in the present work propagation times equal to 450–650 electric field periods, or to about 950–1420 au, were needed until acceptable convergence was achieved. Though huge, the finite size of the lattice does not allow us to exceed the propagation time beyond the above electric field periods due to reflections occurring at the boundaries which generally distort the cross section since it becomes exceptionally large or

small compared to the expected value. Within the degree of accuracy our TDCC calculation does not reveal any noticeable oscillatory structures in the photo-double ionization cross section of ground-state helium near threshold. The same conclusion can be drawn from the experimental cross section data by Kossmann *et al* [8] which are also plotted in figure 1. Their absolute cross section was deduced from the measured ratio of He^{2+}/He^{+} ions by using an already known total photoabsorption cross section [31]. The overall agreement between the TDCC data and the experimental data is very good. Within the measurement inaccuracy their proportionality constant $\sigma_0 = 1.02(4)$ kb agrees well with ours. Slight deviations occur around 2.0 eV excess energy and almost at threshold where the TDCC data may not be fully converged as detailed above. However, more recent measurements of the total photoabsorption cross section of helium [32, 33] give values that are about 6% smaller than those of [31]. Thus, re-scaling the absolute cross section by Kossmann *et al* [8] should result in slightly smaller values and in an even better agreement with our TDCC data.

Realizing that time-dependent close-coupling calculations near threshold are difficult to be carried out and that there might be small oscillations in the photo-double ionization cross section which could not be found yet because they may be below the numerical as well as experimental uncertainties, we have performed another type of calculation by which we can further reduce the numerical uncertainties and get converged results closer to threshold.

This calculation considers a simpler model system which has the same generic properties as the helium atom but only two instead of six spatial degrees of freedom. This is achieved by restricting the angular momenta of the two electrons to be zero and by replacing the electron–electron repulsion in expression (4) by $1/(r_1 + r_2)$ [5]. This model potential is motivated by the observation that close to threshold the two ejected electrons are on opposite sides of the nucleus, i.e. $\hat{r}_1 \approx -\hat{r}_2$. The time-independent Hamiltonian for the helium atom in this so-called *s*-wave counterlinear model reduces to

$$H_{\text{atom}}^{\text{model}} = -\frac{1}{2}\frac{\partial^2}{\partial r_1^2} - \frac{Z}{r_1} - \frac{1}{2}\frac{\partial^2}{\partial r_2^2} - \frac{Z}{r_2} + \frac{1}{r_1 + r_2}. \tag{8}$$

Using this Hamiltonian, the model calculation basically follows equations (2), (3) and (5) but with arguments r_1 and r_2 instead of the vectors. In addition, the Hamiltonian of the classical time-dependent electric field is now written as

$$H_{\text{field}}^{\text{model}} = E(t)(r_1 + r_2)\,\mathrm{e}^{\mathrm{i}\omega t} \tag{9}$$

with the amplitude

$$\begin{aligned} E(t) &= 1/2[1 - \cos(4\pi t/t_{\text{tot}})] \qquad \text{for} \quad t < t_{\text{tot}}/2 \\ E(t) &= 0 \qquad\qquad\qquad\qquad\quad \text{for} \quad t \geqslant t_{\text{tot}}/2. \end{aligned} \tag{10}$$

This choice of amplitude was motivated by the observation that, in the *s*-wave counterlinear model, the photo-double ionization probability converges much faster by using a pulse than an amplitude of the form (7). Thus, the photo-double ionization probability is determined long after the electric field has been turned off.

Regarding numerical aspects of the *s*-wave counterlinear model calculation, equation (5) with the Hamiltonians (8) and (9) and r_1 and r_2 instead of the vectors is propagated in time on a uniform lattice that consists of 3082 × 3082 points. With a mesh spacing of $\Delta r = 0.3$ au this lattice covers an area of 924.6 au × 924.6 au. To better avoid reflections at the boundaries of the lattice caused by those parts of the two-dimensional wavefunction $\Psi^{^1\mathrm{P}}$ which represent single photoionization (see, e.g., [14]), the wavefunction has been multiplied by a mask function whose amplitude decreases from unity to zero over the last 20–30 au of the lattice. This allows us to increase the propagation time which, in turn, results in a well-defined

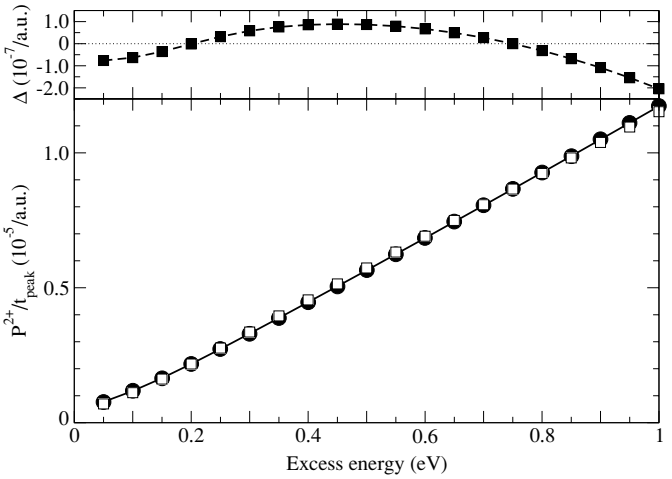

Figure 2. Scaled probability P^{2+}/t_{peak} for photo-double ionization of He ($1s^2\ ^1S$) as a function of the excess energy: □ s-wave counterlinear model data, ● convolved Wannier power law (11) with $P^{2+}_{0.75\,\mathrm{eV}} = 3.8387 \times 10^{-4}$. The upper panel shows the difference Δ (■) between the two data sets.

peak of the Fourier transform of $E(t)$ in the energy space centred around the photon energy (see below). The one-electron wavefunctions of He^+ used for calculating the photo-double ionization probability by means of projection are calculated on a one-dimensional lattice of twice the radial size as the two-dimensional lattice used for time propagation. As the s-wave counterlinear model calculation demands much less computational resources than the time-dependent close-coupling calculation does, much more convergence checks with regard, for example, to lattice size, mesh spacing and total propagation time have been done to further reduce the computational uncertainties.

Figures 2 and 3 show the results of our s-wave counterlinear model calculation for the scaled photo-double ionization probability for the ground state and excited state 1s2s ^1S of helium as a function of the excess energy up to 1.0 eV. Due to the slow convergence, these results are extrapolated probabilities ($t \to \infty$) which have been obtained by fitting the photo-double ionization probability to the expression $A + B(t - t_{\mathrm{peak}})^{-1} + C(t - t_{\mathrm{peak}})^{-2}$ with $t_{\mathrm{peak}} = t_{\mathrm{tot}}/4$ for the last quarter of the total propagation time $t_{\mathrm{tot}} = 1800$ au. A series of calculations have been done using lattices of $1/4$ and $1/2$ the size of the final lattice. We find the scaled photo-double ionization probability for the ground state to be about an order of magnitude smaller than that for the excited singlet state. This goes on for energies beyond the near-threshold region, e.g. [16, 23]. Scaled by t_{peak}, the full circles refer to a convolved Wannier power law given by

$$P^{2+} = P^{2+}_{0.75\,\mathrm{eV}} \frac{\langle E^{\alpha}_{\mathrm{exc}} \rangle_E}{\langle E^{\alpha}_{\mathrm{exc}} \rangle_{0.75\,\mathrm{eV}}}, \tag{11}$$

where

$$\langle E^{\alpha}_{\mathrm{exc}} \rangle_E = \frac{\int_0^{\infty} \mathrm{d}E \left| \mathcal{F}\left(E - E^{\alpha}_{\mathrm{exc}}\right) \right|^2 E^{\alpha}}{\int_{-\infty}^{\infty} \mathrm{d}E \left| \mathcal{F}\left(E - E^{\alpha}_{\mathrm{exc}}\right) \right|^2} \tag{12}$$

and $\mathcal{F}$ is the Fourier transform of the pulse amplitude defined by equation (10). For the photo-double ionization probabilities at 0.75 eV excess energy, our s-wave counterlinear model

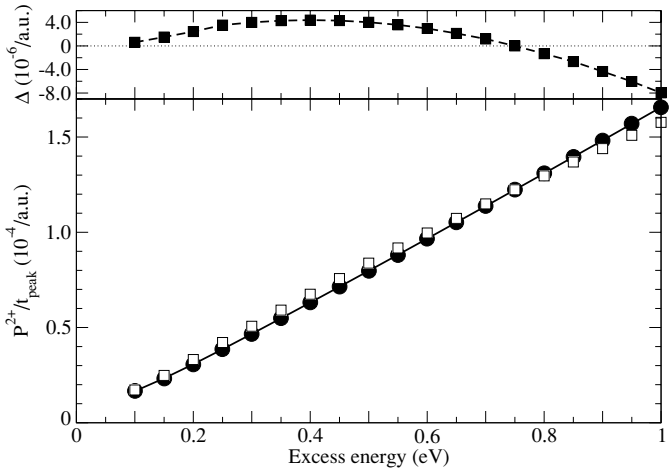

Figure 3. Scaled probability P^{2+}/t_{peak} for photo-double ionization of He (1s2s ^{1}S) as a function of the excess energy: □ s-wave counterlinear model data, ● convolved Wannier power law (11) with $P^{2+}_{0.75\,\mathrm{eV}} = 5.4223 \times 10^{-3}$. The upper panel shows the difference Δ (■) between the two data sets.

calculation yields $P^{2+}_{0.75\,\mathrm{eV}} = 3.8387 \times 10^{-4}$ for the ground state and $P^{2+}_{0.75\,\mathrm{eV}} = 5.4223 \times 10^{-3}$ for the excited singlet state. By employing a convolved Wannier power law, we account for the energy distribution centred around the actual photon energy as a result of the finite time the electric field given by the relations (9) and (10) is kept on. The longer the electric field is kept on, the smaller are the contributions of other energies of the distribution to the photo-double ionization probability. However, this time is limited since time is also needed for the development of the wavefunction after the electric field has been turned off before accurate projections can be carried out. The overall time, in turn, is limited by the size of the lattice. As is evident from figure 2, the scaled probabilities for photo-double ionization of ground-state helium almost match the scaled and convolved Wannier power law over the entire energy region. The deviation of the scaled probabilities from the Wannier curve is shown in the upper panel of figure 2 and is about two orders of magnitude smaller. At a first glance the deviation may be due to numerical inaccuracies as neither in magnitude nor in period do they resemble the oscillatory structures that have been found for the photo-double ionization cross section of lithium [6] and beryllium [7]. However, taking into account the excited singlet state of helium and observing that the deviation of the scaled probabilities from the Wannier curve is just one magnitude smaller (see the upper panel of figure 3) and thus much larger than for the ground state, other reasons for these deviations are more likely than numerical inaccuracies. Almost at threshold the deviations may be especially due to the pulse width and projections while at higher energies inclusion of higher-order terms in the Wannier law may be of importance. Nonetheless, we do not consider these deviations as oscillations. It is clear that for the excited singlet state of helium, the validity of the lowest-order Wannier theory is restricted to smaller excess energies than for the ground state. Taking the classical picture of the Wannier theory into account, it is more likely for the ground state than for the excited singlet state with a 1s and a 2s electron that the electrons will leave the atom from almost the same distance to the nucleus and with almost the same kinetic energies. But the larger deviations may also have something to do with the model system used, since restricting all angular momenta of the two electrons to zero is more appropriate for the ground state than for excited states.

In conclusion, for the first time, an *ab initio* non-perturbative calculation has generated absolute data for the near-threshold photo-double ionization cross section of ground-state helium below 1.0 eV which are in excellent agreement with the pioneering measurement by Kossmann *et al* [8]. The calculation supports the Wannier power law up to about 1.7 eV excess energy and provides the proportionality constant, which is $\sigma_0 = 0.998$ kb. Within the accuracy of the calculation the photo-double ionization cross section does not show any oscillatory behaviour near threshold. The *s*-wave counterlinear calculation, which considers a simpler model system but allows for a significant reduction of numerical uncertainties also does not reveal any oscillations, neither for the ground state nor for the additionally investigated lowest-excited singlet state of helium.

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