Positronium-dipole induced resonances in $e^+$-H and $e^+$-alkali systems

M Umair and S Jonsell

Department of Physics, Stockholm University, SE-10691 Stockholm, Sweden

E-mail: muhammad.umair@fysik.su.se and jonsell@fysik.su.se

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Abstract

We derive general universal scaling relations governing resonances induced by the dipole moment of excited positronium interacting with atomic ions. A single non-universal parameter, which contains all the system-dependent information, is defined. Our results are compared to numerical calculations, using complex scaling, for $S$, $P$, and $D$-wave resonances below the positronium $n = 2$ threshold in the $e^+$(H, Li, Na, K) systems. The energy and width ratios of the successive resonances are found to agree well with the analytically derived scaling law.

Keywords: positronium, resonances, dipole series, three-body systems

(Some figures may appear in colour only in the online journal)

1. Introduction

Universal phenomena, i.e. phenomena which are independent of the system studied, or whose dependence can be captured by only a small number of parameters, has recently received a lot of attention within atomic physics, and related fields. Examples are ultracold atom–atom interactions which can be described by the scattering length alone, and as a consequence, a large number of phenomena associated with normal or quantum gases can be described using the scattering length as the only parameter. In the three-particle sector Efimov derived a universal attractive interaction of $r^{-2}$ form which supports bound states, with energies depending only on the scattering length and one additional parameter [1–3]. The signature of such states in clouds of ultracold Cs-atoms [4] opened the door to the a surge of activity, both experimental [5–8] and theoretical [9, 10], on universal properties of few-atom systems.

Another system featuring an attractive $r^{-2}$ potential is the interaction of a dipole with a charged particle. While molecules may have large electric dipole moments, the spherical symmetry normally forbids this in atoms. The exception is excited states of the hydrogen atom, where similar universal physics has been invoked, in particular, to interpret the structure of resonances in H$^+$ as an electron interacting with the dipole of an H($n = 2$) state [11]. Another charged particle which in a similar way may interact with excited hydrogen is the positron. Mittleman pointed out that the positron-hydrogen system should, therefore, contain an infinite sequence of dipole resonances [12]. Since then, a large number of numerical studies have further investigated such positron-hydrogen resonances [13–20].

The reason why the hydrogen atom is unique is that it has energy levels which are degenerate with respect to orbital angular momentum (all relativistic effects are neglected in this work). Then the interaction with a charged particle will perturb the spherical symmetry in such a way that a dipole is induced. Since the states are degenerate, there is no energy cost for this process, i.e. it is a real, not virtual effect (in the sense of quantum mechanics). This is in contrast to other atoms with non-degenerate energy levels, which may be coupled only as a second-order effect, where states with higher energy are required as virtual intermediary states. Thus, this polarisability of the atom instead gives an attractive $1/r^4$ interaction.

There is, however, another atom-like system with degenerate energy levels; positronium (Ps)—the bound state of an electron and a positron. As was pointed out in [21, 22], the mass scalings of Ps are favourable, giving more closely
spaced, and hence larger numbers of dipole states, as compared to hydrogen. In \( e^+ - A \) scattering (A stands for any atom) the Ps-A\(^+\) configuration will arise as a possible channel. Thus the \( 1/r^2 \) potential is supported by the dipole moment of a projectile rather than, as in \( e^+ - H \) scattering, the target.

A number of theoretical studies of resonances in the positron-alkali system have been conducted [22–31]. Apart from having non-degenerate \( l \)-levels, and thus no sequences of dipole states converging to the atomic thresholds, the alkali systems also differ from hydrogen in other ways. Firstly, the alkali atoms have large dipole polarisabilities that sometimes are strong enough to produce truly bound atom-\( e^+ \) states [21]. Secondly, in \( e^+ - \)alkali collisions the positronium formation channel is open all the way down to zero energy. Ward et al [23] were the first to carry out calculations using the five-state close-coupling method in \( e^+ - \)alkali systems. However, no Ps formation channel was included in their calculations. Kar and Ho [24] applied the stabilisation method to evaluate the resonances in \( e^+ \)- (Na, K) systems. They used Hylleraas-type wavefunctions to represent the correlation effects between the valence electron, the positron, and the core. Han et al [25, 26] also applied the stabilisation technique to evaluate resonances in \( e^+ \)-(Na, Li) systems using hyper-spherical coordinates. Both these calculations were limited to only \( S \)-wave symmetry. Liu and Jiao [27, 28] studied higher partial waves in \( e^+ \)-(Li, Na) systems using the momentum space coupled-channel optical method. In these works, only a few \( S, P, \) and \( D \)-wave resonances were reported below the Ps(\( n = 2 \)) threshold.

In a recent sequence of studies, we have applied a computational scheme to calculate resonances for the three-body systems using the complex scaling method applied to explicitly correlated Gaussian trial functions [20, 22, 29–31]. This has proved to be an effective method to calculate resonances, and we have been able to find many more resonances than had been reported previously. Here we update our results from these works with more complete and accurate sequences of resonances below the Ps(\( n = 2 \)) threshold.

The objective of the current study is to provide a general and detailed analytical analysis of the dipole sequences in \( e^+ - H \) and \( e^+ - \)alkali systems, and present this analysis side by side with our best numerical results for the \( n = 2 \) threshold. From this, we try to draw some general conclusions about the nature of these dipole sequences, as well as noting their differences. In particular, we find that the differences to some extent can be summarised in a single parameter, which also governs the low-energy Ps-\( A^+ \) scattering above the thresholds.

We start in section 2 by providing a general derivation of the analytical scaling relations for the dipole series. In section 3 we extend this formalism to scattering states above the thresholds. In section 4 we give a brief account of the numerical method we have used. Then in section 5 we try to couple the numerical results thus obtained back to the analytical formalism. Finally, we draw conclusions in section 6.

Atomic units are used unless otherwise is specified.

2. Dipole series

We here derive the dipole potential for Ps(\( n = 2 \)) interacting with a charged particle, such as an ionic core. The derivation follows closely that of Temkin and Walker [111], but has been generalised to arbitrary angular momenta and Ps-states, as well as adapted to Ps rather than hydrogen. A shortened version of this derivation has been presented in the appendix of [22].

We start by expanding the wavefunction in the complete set of Ps-states \( \psi_{\text{in}}(r) = R_{\text{in}}(r) Y_{\text{in}}(\hat{r}) \) as

\[
\psi(r, \rho) = \sum_{n,l,l',\ell,\ell'} f_{nll\ell\ell'}(\rho) R_{\text{in}}(r) [Y_l(\hat{r}) \otimes Y_{\ell}(\hat{\rho})] Y_{\ell'}(\hat{\rho}),
\]

where \( r \) and \( \rho \) are the internal and the centre-of-mass coordinates of positronium, \( \{ J, M \} \) the total orbital angular momentum of the system, \( L \) the orbital angular momentum of the Ps centre-of-mass motion, and

\[
[Y_l(\hat{r}) \otimes Y_{\ell}(\hat{\rho})] Y_{\ell'}(\hat{\rho})] = \sum_{l',m} (lM_l|M_{l'}) Y_{\ell m}(Y_{\ell'}(\hat{\rho}) Y_{\text{in}}(r) Y_{\text{in}}(\hat{r}), \rho) \]

with \( (lM_l|M_{l'}) \) the Clebsch–Gordan coefficient. Spin functions are not included in this derivation, as relativistic effects are ignored, and there are no identical particles except the electrons inside the atomic core (that is, exchange between the electron inside Ps and the electrons inside the core is neglected). The sum in (1) is restricted to terms for which \((-1)^{l+\ell+\ell'} = 1 \) (1) for natural (unnatural) parity states.

The Hamiltonian can be written as

\[
\hat{H} = \hat{H}_{\text{Ps}} - \frac{1}{2M} \Delta_{\rho} + V(r, \rho),
\]

where

\[
V(r, \rho) = \frac{1}{|\rho - r/2|} - \frac{1}{|\rho + r/2|}
\]

is the Coulomb interaction between the Ps and the core. \( \hat{H}_{\text{Ps}} \) is the Hamiltonian for Ps, and \( M = 2 \) is the Ps mass. Projection of the Schrödinger equation with \( \psi_{\text{in}}(r) Y_{\ell M}(\hat{\rho}) \) gives an infinite set of coupled equations,

\[
\left\{ \begin{array}{l}
- \frac{1}{2M} \frac{\partial^2}{\partial \rho^2} + \frac{L(L + 1)}{2M \rho^2} - \varepsilon_{\ell M} \left[ \langle lM_l|M_{l'} \rangle Y_{\text{in}}(r) Y_{\text{in}}(\hat{r}) \right] \\
+ \sum_{l'=l-1}^{l+1} \sum_{l''} \langle l'l''M_l|M_{l'} \rangle Y_{\text{in}}(r) Y_{\text{in}}(\hat{r}) \\
\times \int \psi_{\text{in}}^{*}(r) Y_{\ell M}(\hat{\rho}) V(r, \rho) Y_{\ell' M}(\hat{\rho}) \right. \\
\times \left. \psi_{\text{in}}^{*}(r) Y_{\ell' M}(\hat{\rho}) \right) \right. \\
\end{array} \right.
\]

where \( \ell \) and \( L \) are restricted by the inequalities \( |l - L| \leq \ell \leq l \), \( l \leq n - 1 \) and \((-1)^{l+L} \) gives the desired parity of the state. Here \( \varepsilon_{\ell M_l} \) is the collision energy relative the Ps(\( n \)) threshold, i.e., the total energy satisfies \( E = \varepsilon_{\ell M_l} + \varepsilon_{\text{Ps}}, \) where \( \varepsilon_{\text{Ps}} \) is the energy of the Ps states with principal quantum number \( n \), and \( \nu \) denotes successive states.
in the dipole series. Now, use the fact that
\[ \sum_{m,J} \langle \{LmM_l|JM_j\}^2 = \frac{2J + 1}{2L + 1} \]
to get the more convenient form
\[ \left( - \frac{1}{2M} \frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{L(L + 1)}{2M r^2} - \varepsilon_{nl\mu} \right) f_{nLlJ\mu}(r) + \frac{2L + 1}{2J + 1} \times \sum_{m,J} \langle \{LmM_l|JM_j\} \sum_{n',l',M'_{l'}} \langle l' l'M'_{l'}|JM_{J'} \rangle \times \int \psi_{n'm'}^* (r) Y_{LM}^* (\hat{r}) \psi_n (r) Y_{LM} (\hat{r}) \mathrm{d}r \mathrm{d}\Omega \rho \times \psi_{n'm'} (r) \mathrm{d}r \mathrm{d}\Omega \rho = 0. \]
(6)

We now proceed to study this equation for energies close to the threshold energy, i.e. for small \( \varepsilon_{nl\mu} \).

### 2.1. Short-distance solution

This is the range where \( \varepsilon_{nl\mu} \) can be neglected compared to the potential \( V(r, \rho) \). The size of this region will increase if \( \varepsilon_{nl\mu} \) is sufficiently small. The solution in this region is thus energy-independent, and as we shall see this is the key to getting a sequence of resonance with a universal scaling of their energies.

### 2.2. Long-distance solution

The long-range region is defined by the validity of two approximations.

1. The interaction \( V(r, \rho) \) can be replaced by its long-range form, that is
\[ V(r, \rho) \approx \frac{4\pi}{3} \frac{r}{\rho^2} \sum_{\mu = -1}^1 \frac{1}{\rho^3} \left| Y_{\mu} (\hat{r}) Y_{\mu}^* (\hat{r}) \right|, \]
(7)
The condition for the validity of this approximation is simply \( \rho \gg r \). The maximum of \( r \) is limited by the extent of the probability density of Ps, which is exponentially damped as \( \exp(-r/n) \). Thus we require \( \rho \gg n \). When this condition is satisfied the interaction term in (6) simplifies to
\[ \frac{4\pi}{3} \frac{1}{\rho^2} \sum_{m,J} \langle \{LmM_l|JM_j\} \times \sum_{n',l',M'_{l'}} \langle l' l'M'_{l'}|JM_{J'} \rangle \times \int \psi_{n'm'}^* (r) Y_{LM}^* (\hat{r}) \psi_n (r) Y_{LM} (\hat{r}) \mathrm{d}r \mathrm{d}\Omega \rho \times \psi_{n'm'} (r) \mathrm{d}r \mathrm{d}\Omega \rho = \mathbf{0}. \]
(8)

Next, use that
\[ \int \psi_{n'm'} (r) \mathrm{d}r \mathrm{d}\Omega \rho = (-1)^m, \]
\[ \int \psi_{n'm'} (r) \psi_n (r) \mathrm{d}r \mathrm{d}\Omega \rho = \mathbf{0}, \]
to evaluate the integrals in (8). We then get, after using some standard symmetry relations for the Clebsch–Gordan coefficients,
\[ \frac{1}{\rho^2} \sum_{n', l'} \langle \{R_{n'l'}|R_{n'l'} \rangle \sum_{M_{J'}} (-1)^{J + L + L'} \times \frac{2L + 1}{2J + 1} \times \sum_{m,J} \langle \{JmM_l|JM_j\} \times \langle l' l'M'_{l'}|JM_{J'} \rangle \times \langle \{LmM_l|JM_j\} \times \langle l' l'M'_{l'}|JM_{J'} \rangle \times \langle \{R_{n'l'}|R_{n'l'} \rangle \sum_{M_{J'}} (-1)^{J + L + L'} \]
\[ \mathbf{0}. \]
(9)

(2) We see from above that in the large \( \rho \) regime, the interaction term approaches zero as \( V \propto \rho^{-2} \), and may thus be treated as a perturbation compared to the overall energy scale set by the Ps-energies \( E_0 \). The problem is then properly treated by degenerate-state perturbation theory. Accordingly, to leading order only states with the same \( n \) quantum number are coupled, with the coupling of order \( V \). Couplings between different \( n \)'s will be second order, proportional to \( V^2/(E_0 - E_{n+1}) \approx 2n \rho^2 \). Requiring that these terms are much smaller than \( V \), we arrive at the condition \( \rho \gg n^{1/2} \), which is stronger than the one above under (1). For values of \( \rho \) satisfying this condition the infinite sum over \( n' \) in (6) can be collapsed to a single term \( n' = n \) (that is, we only include couplings between degenerate Ps states).

We then finally arrive at the coupled equations,
\[ \left( - \frac{1}{2M} \frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{L(L + 1)}{2M r^2} - \varepsilon \right) f_{nLlJ\mu}(r) \]
\[ - \frac{1}{\rho^2} \sum_{n', l'} \sum_{M_{J'}} (-1)^{J + L + L'} \mathrm{D}_{n' \rho}(\rho) \times \sqrt{(2L + 1)(2L' + 1)} \langle \{R_{n'0}\} \langle \{L00\} \rangle \sum_{JL} \langle \{R_{n'l'}|R_{n'l'} \rangle \sum_{M_{J'}} (-1)^{J + L + L'} \times \sum_{m,J} \langle \{JmM_l|JM_j\} \times \langle l' l'M'_{l'}|JM_{J'} \rangle \times \langle \{R_{n'l'}|R_{n'l'} \rangle \sum_{M_{J'}} (-1)^{J + L + L'} \]
\[ \mathbf{0}. \]
(10)
The expression (10) is a system of equations, coupled by the interaction term. Diagonalising the effective interaction (including the angular momentum barrier) both positive and negative roots may be obtained. Any negative roots will give rise to an attractive effective potential, supporting a dipole series of states (in this case meta-stable states, or resonances, since they are embedded in the continuum of ground-state Ps, as well as atom + positron continua of a number of atomic states). Denoting such an attractive effective interaction by \(-\lambda/\rho^2\), the long-range form of the Schrödinger equation is

\[ \left( -\frac{1}{2M} \frac{\partial^2}{\partial \rho^2} - \frac{\lambda}{\rho^2} \right) f(\rho) = \varepsilon f(\rho), \tag{11} \]

where \( f(\rho) \) is the linear combination of the \( f_{m=0}^{\nu} \) corresponding to the appropriate eigenfunction of the potential matrix. The analytic form of the solution which is finite as \( \rho \to \infty \), can be found as

\[ f(\rho) = \sqrt{\kappa \rho} H_1^{(1)}(\i\kappa \rho), \quad \kappa = \sqrt{-2M\varepsilon}, \tag{12} \]

where, \( H_1^{(1)} \) is the Hankel function of the first kind, and

\[ \alpha = \sqrt{1 - 4 + 2ML}. \tag{13} \]

It should be noted that the solution (12) was derived only from the properties of Ps. Hence, the result does not depend on any property of the atom. It is universal, in the sense that it is the same for any alkali ion (or proton) interacting with positronium.

### 2.3. Matching the solutions

Equation (12) gives a long-range solution for any energy \( \varepsilon \). In order to select the correct quantised solutions we have to match the short-range and long-range solutions at some \( \rho = \rho_m \). For this to work there has to be some region where both solutions are valid, and \( \rho_m \) has to be chosen within this region (though for our purposes it is enough to establish that such a \( \rho_m \) does exist, its value is of no consequence). As derived above, the long-range solution is valid if \( \rho \gg n^{1/2} \), while the energy-independent short-range solution is valid if \( |\varepsilon| \ll |V| \sim \rho^{-2} \). These two conditions are not mutually exclusive as long as \( |\varepsilon| \ll n^{-3} \). We can thus find a matching distance satisfying \( n^{1/2} \ll \rho_m \ll |\varepsilon|^{-1/2} = \sqrt{2M}/\kappa \).

Since \( \sqrt{2M} \) is of order unity (actually \( \approx 2 \) for Ps), we can from the condition above derive that \( \kappa \rho_m \ll 1 \). At this argument the short-range approximation to the Hankel function in (12) can be used, giving

\[ f(\rho_m) \approx \frac{2\rho_m^{1/2}}{[\alpha \pi \sinh(\alpha \rho_m)^{1/2}]} \sqrt{\kappa \rho_m} \sin[\alpha \ln(\kappa \rho_m/2) - \varphi], \tag{14} \]

where \( \varphi = \arg[\Gamma(1+i\alpha)] \), and \( \alpha \) was defined above in (13).

The matching of the solutions at \( \rho = \rho_m \) is done by setting their log-derivatives equal. We do not actually know the log-derivative of the short-range solution, but that doesn’t matter. The important thing is that it does not depend on energy, and thus is the same for all the states in the dipole series. We call it \( K \), and hence from equation (14),

\[ K = \frac{f'(\rho)}{f(\rho)} \bigg|_{\rho=\rho_m} = \frac{1}{2\rho_m} \left( 1 + 2 \cot \left[ \alpha \ln \kappa \rho_m \right] - \varphi \right). \tag{15} \]

The energy-independence of \( K \) gives rise to the dipole series. As we shall see, this series has universal properties because the long-range form of the wavefunction is the same for all atoms. However, \( K \) in itself is non-universal since it depends on the short-range physics, which is going to be different for different atoms. This means that the location of the resonances is not going to be completely determined.

We could use (15) to solve for \( \kappa \) and thus determine the quantised energies. Then we find the reason why we get an, in principle, infinite number of states. The cause lies in the periodicity of the \( \cot \alpha \) function, for which a given \( K \) will give an infinite number of solutions for \( \kappa \). Any of these values of \( \kappa \) could then be used in (12) giving a long-range wavefunction depending, like \( \kappa \), on \( K \rho_m \). It would seem then that the solution depends on the choice of \( \rho_m \), but as we have seen above this should not be the case, as long as \( \rho_m \) is chosen within the appropriate bounds. The value of \( K \) thus has to vary with \( \rho_m \) in such a way that the same solution is obtained for all \( \rho_m \). Using \( K \) as the parameter for the matching thus obscures the full universality of the solutions. We therefore introduce in its place another parameter \( \Lambda_0 \), defined such that the matching radius, i.e. for \( n^{1/2} \ll \rho \ll \kappa^{-1} \)

\[ f(\rho) = N\sqrt{\rho} \sin[\alpha \ln(\rho \Lambda_0)], \tag{16} \]

with \( N \) some normalisation constant which is unimportant. From this we derive the relation between \( \Lambda_0 \) and \( K, \rho_m \) as,

\[ \kappa \rho_m = 1 + \alpha \cot[\alpha \ln(\rho_m \Lambda_0)], \tag{17} \]

or

\[ \Lambda_0 = \frac{1}{\rho_m} \exp \left[ \frac{1}{\alpha} \cot^{-1} \left( \frac{1}{\alpha} (K \rho_m - 1/2) \right) \right]. \tag{18} \]

The parameter \( \Lambda_0 \) captures the co-variation of \( K \) and \( \rho_m \), and combines them into a single parameter. This parameter is still non-universal in the sense that it is different for different atoms. Note that \( \Lambda_0 \) has dimension of inverse length, when we give numerical values atomic units will be used, but it could of course be referred to any length scale.

Since \( \Lambda_0 \) appears inside a periodic function its relation to states of the system is not one-to-one. To explore this we write the relation between \( \Lambda_0 \) and \( \kappa, \rho_m \), by comparing equations (14) and (16), which gives for \( \nu = 0, 1, 2, 3, … \)

\[ \alpha \ln \Lambda_0 \rho_m - \nu \pi = \alpha \ln \frac{\kappa \rho_m}{2} - \varphi, \]

or \( \kappa = 2\Lambda_0 \exp(-\nu \pi/\alpha + \varphi/\alpha) \). Hence, the final result for the energy as a function of \( \Lambda_0 \) is

\[ \varepsilon_{\nu,\nu} = -2\Lambda_0^2 \frac{1}{M} \exp \left\{ \frac{2}{\alpha} (\varphi - \nu \pi) \right\}, \tag{19} \]

where the subscript \( \nu \) denotes different states in the series.
The energy-scaling between consecutive dipole states is
\[ \frac{\varepsilon_{nJ,\nu}}{\varepsilon_{nJ,\nu + 1}} = \frac{2\pi}{\varepsilon_{nJ,\nu + 1}}, \tag{20} \]
which is independent of \( \Lambda_0 \) and hence the same for all alkalis, i.e. universal. The scaling relation still depends on \( \alpha \) and will therefore be different for different thresholds \( n \) and total angular momenta \( J \). In [22] we presented a table of \( \alpha \) for different \( n \) and \( J \). It should be noted that Ps (\( M = 2, \mu = 1/2 \)) and \( \text{H}(M = \mu = 1) \) differ only by the masses. Both mass factors work in the same direction, i.e. to increase \( \lambda_+ \) and \( \alpha \) for Ps as compared to H. Thus, for Ps the dipole states lie closer in energy and the dipole approximation can be expected to be valid over a wider range. Both effects increase the number of dipole states.

2.4. Example, the \( n = 2, J = 0 \) threshold

As an example we calculate the scaling relation for \( n = 2 \) and \( J = 0 \). We can write the wavefunction at large Ps-A\(^+\) separations \( \rho \) as
\[
\Psi(\vec{r}, \vec{p}) = \frac{1}{\rho} f_{200,0}(\rho) R_{2s}(r) |Y_0(\vec{p}) \otimes Y_0(\vec{p})\rangle_{00} + \frac{1}{\rho} f_{201,0}(\rho) R_{2p}(r) |Y_1(\vec{p}) \otimes Y_1(\vec{p})\rangle_{00}, \tag{21} \]
where \( R_{2s}(r) \) and \( R_{2p}(r) \) are the radial wavefunctions of the hydrogen-like 2s and 2p states of Ps.

We proceed by inserting the form (21) for \( \Psi \) in the Schrödinger equation, and project with the 2s and 2p states of Ps. This gives the coupled equations
\[
\left( -\frac{1}{2M} \frac{\partial^2}{\partial \rho^2} - \varepsilon_{2s,0}(\rho) \right) f_{200,0}(\rho) = \frac{3}{\mu} \frac{1}{\rho^2} f_{202,0}(\rho),
\]
\[
\left( -\frac{1}{2M} \frac{\partial^2}{\partial \rho^2} + \frac{1}{M \rho^2} - \varepsilon_{2s,0}(\rho) \right) f_{202,0}(\rho) = \frac{3}{\mu} \frac{1}{\rho^2} f_{200,0}(\rho). \tag{22} \]

Here \( \mu = 1/2 \) is the reduced mass of Ps (note that for H the expression is the same except that \( M = \mu = 1 \)). The coupled equations can be rewritten as
\[
-\frac{1}{2M} \frac{\partial^2}{\partial \rho^2} \left( f_{200,0}(\rho) - \frac{1}{\rho} f_{202,0}(\rho) \right) = \varepsilon_{2s,0}(\rho),
\]
\[
\left( f_{202,0}(\rho) - \frac{1}{\rho} f_{200,0}(\rho) \right) = \varepsilon_{2s,0}(\rho), \tag{23} \]
where \( \varepsilon_{2s,0}(\rho) = \frac{1}{\rho^2} \left( 6 - \frac{1}{2} \right) \). Diagonalising this matrix gives two roots: \( \lambda_+ = \frac{1}{4} (1 \pm \sqrt{577}) \). The root \( \lambda_+ \) gives a repulsive potential, while the root \( \lambda_- \) gives the attractive potential
\[
V_-(\rho) = \frac{377}{4\rho^2}.
\]
Thus we have for \( n = 2 \) and \( J = 0 \) the potential given by \( \lambda_+ = 5.755 \). Comparing to equations (13) and (20) we have \( \alpha = 4.772 \) and \( \varepsilon_{2s,0}/\varepsilon_{2s,0+1} = 3.73 \). Below we shall compare this analytical result to numerical calculations for different atoms.

3. Scattering

The formalism developed in the preceding section is valid also for energies just above the threshold. It can thus also be applied to low-energy scattering of excited Ps on alkali ions. The difference is that there is no requirement that the wavefunction vanishes at large distances, so rather than just the single solution (12) in the long-range region, we now get two linearly independent solutions, i.e.
\[
f(\rho) = \sqrt{\rho} (C_1 H_{2s}^1(\rho \rho) + C_2 H_{2s}^2(\rho \rho)), \tag{24} \]
where \( k = \sqrt{2M\varepsilon} \). These functions may be regarded as eigenfunctions of complex angular momentum \( I = i\alpha - 1/2 \) (then \( I(l + 1) = -\alpha^2 - 1/4 = -2M\lambda \) in agreement with (11) and (13)). We can determine the constants \( C_1 \) and \( C_2 \) by again matching to the form (16) at \( \rho \ll \varepsilon^{-1/2} \). We then need the short-range form of the Hankel functions (now for real arguments), which gives
\[
f(\rho_{\text{in}}) = \sqrt{\rho_{\text{in}}} \left( \frac{\sin \pi \alpha}{\pi \alpha} \right) \left( 1 + \frac{\cosh \pi \alpha}{\sin \pi \alpha} \right) e^{i(\alpha \ln(k_0^2/2) - \varphi)}
\]
\[
- \frac{1}{\sin \pi \alpha} e^{-i(\alpha \ln(k_0^2/2) - \varphi)}
\]
\[
+ C_2 \left( 1 - \frac{\cosh \pi \alpha}{\sin \pi \alpha} \right) e^{i(\alpha \ln(k_0^2/2) - \varphi)}
\]
\[
+ \frac{1}{\sin \pi \alpha} e^{-i(\alpha \ln(k_0^2/2) - \varphi)}. \tag{25} \]

Since we have two undetermined parameters \( C_1 \) and \( C_2 \), matching to (16) is here possible for all \( k \), and will give the ratio \( C_2/C_1 \) as a function of \( k \) and \( \Lambda_0 \). The condition becomes
\[
C_2/C_1 = \frac{1 - e^{2i\varphi}}{1 - e^{2\varphi} - 2\varphi}. \tag{26} \]

where \( \eta = \alpha \ln(k/(2\Lambda_0)) - \varphi \). We cannot directly identify this result with the scattering phase shift, because the Hankel functions of imaginary order are exponentially growing or declining. Using the asymptotic forms of the Hankel functions in (24) together with the result (26) we find that
\[
f(\rho) \rightarrow N' \left( e^{-ik_0\rho - \pi/4} - e^{2i(\eta + \pi) \rho - \pi/4} \right) \text{ as } \rho \rightarrow \infty, \tag{27} \]

where \( \sigma = \tan^{-1} \left( \frac{\sin 2\eta}{\exp(\pi x) - \cos 2\eta} \right) \approx e^{-\alpha \pi} \sin 2\eta \). The simplification of \( \sigma \) assumes that \( e^{\alpha \pi} \gg 1 \), in which case the contribution from \( \sigma \) is very small. We can read off the usual scattering phase shift as
\[
\delta = \eta + \sigma = \alpha \ln(k/(2\Lambda_0)) - \varphi + \sigma. \tag{28} \]

We find a logarithmic variation of the phase shift close to the threshold. Interestingly, the non-universal parameter \( \Lambda_0 \) sets the scale for the energy variation.

As we shall see below, since we are dealing with resonances of a finite life time the parameter \( \Lambda_0 \) is complex. Neglecting \( \sigma \) we then have
\[
\delta_r = \text{Re} \{\delta\} = \alpha \ln(k/(2\Lambda_0)) - \varphi, \tag{29} \]
\[ \delta_i = \text{Im} \{ \delta \} = -\alpha \arg \{ \Lambda_0 \}. \]  

(30)

It must be kept in mind here that \( f(\rho) = f_\alpha(\rho) \) and hence \( \delta = \delta_\alpha \) applies only to the eigenfunction corresponding to the eigenvalue \( \lambda_\alpha \) of the attractive potential, which was obtained when the interaction potential is diagonalised, but not the root giving a repulsive potential (for high thresholds there could also be several attractive potentials). This will not be a single Ps-states, but some linear combination of degenerate Ps-states. Taking the example \( n = 2 \), \( J = 0 \) again, the linear combination giving the eigenfunctions of the potential are

\[ |-\rangle = c_1|2s\rangle + c_2|2p\rangle, \]

\[ |+\rangle = c_1|2s\rangle - c_2|2p\rangle, \]

with \( c_1 = 0.72 \) and \( c_2 = 0.69 \).

The solution \( f_\alpha(\rho) \), corresponding to the repulsive potential \( V_\alpha(\rho) = (1 + \sqrt{\frac{577}{\rho^2}}) / 4\rho^2 \), does not depend on \( \Lambda_0 \) since for small energies the Ps will be reflected by the potential before reaching the short-range region. Its phase shift is therefore much easier to calculate. The solution which is regular as \( \rho \to 0 \) is

\[ f_\alpha(\rho) = \frac{\sqrt{\rho}}{ \sqrt{r_\alpha}} J_{\xi+1/2}(k\rho), \]

(33)

where \( \xi = \sqrt{1/4 - 2\lambda_\alpha} = 1/2 = i\alpha_+ - 1/2 \) (where \( \alpha_+ \) is the analogue of \( \alpha \) but with \( \lambda_\alpha \) replaced by \( \lambda_+ \)). From the long-range form of the Bessel function we then find that \( \delta_\alpha = -\xi\pi/2 \).

Taking for instance the 2s state of Ps we have from (31) and (32) the incoming wave

\[ e^{-i\rho}\langle 2s \rangle = c_1 e^{-ik\rho} \langle - \rangle + c_2 e^{-i2k\rho} \langle + \rangle. \]

(34)

After the collision this has transformed to the outgoing wave

\[ e^{i\rho}(c_1 e^{i2k\rho} \langle - \rangle + c_2 e^{i2k\rho} \langle + \rangle) = e^{i\rho}[1(2e^{i2k\rho} + c_1^2 e^{i2k\rho})|2s\rangle + c_1 c_2 (e^{2i\rho} - e^{2i2k\rho})|2p\rangle] \]

\[ = e^{i\rho+\delta_+}\chi \{(c_1^2 + c_2^2)\cos \chi + i(c_1^2 - c_2^2)\sin \chi \}|2s\rangle + 2i c_1 c_2 \sin \chi |2p\rangle, \]

(35)

where \( \chi = \delta_+ - \delta_\alpha \). Thus we obtain the scattering amplitude for e.g. Ps(2s) to Ps(2p) as

\[ f_{2s\to 2p} = 2i c_1 c_2 e^{i(\delta_+ + \delta_\alpha)} \sin \chi. \]

(36)

Scattering amplitudes for other processes, such as elastic scattering and reactive scattering can be calculated in a similar way.

4. Numerical method

Both systems \( e^+ - H \) and \( e^+ - A \) consist of a positron, an electron, and a nucleus, either a proton or core \( A^+ \). The total Hamiltonian \( \hat{H} \) for the system with the energy expressed in atomic units (a.u.) is given by

\[ \hat{H} = -\frac{1}{2} \nabla_1^2 - \frac{1}{2} \nabla_2^2 + V(\gamma\gamma)(r_1) + V(\sigma\sigma)(r_2) - \frac{1}{r_{12}}, \]

(37)

where the indices 1 and 2 refer to the coordinates of the electron and positron respectively; \( r_{12} \) is the relative distance between them, \( V(\gamma\gamma) \) and \( V(\sigma\sigma) \) are the interaction potentials between the core and the valence electron and the positron respectively.

For the \( e^+ - H \) system the inter-particle interactions are simply Coulombic, but for the \( e^+ - A \) systems we use model potentials for the interaction of the outer electron and the positron to the core. We have used previously tested model potentials, all containing free parameters with values chosen to reproduce atomic energies. We have plotted the screening potential \( S(r) = \sqrt{V(\gamma\gamma)}(r) + 1 \) for different alkali atoms in figure 1. For \( e^+ - Na \) we used the model potential that we employed in our previous study [22]. For \( e^+ - Li \) we used the same model potential as Kar used [24], whereas for \( e^+ - Li \) we used a model potential similar to the one that Han et al [26] employed in their study.

The Schrödinger equation was solved using the coupled rearrangement channels method developed by Kamimura and co-workers [33, 34]. The three-body wavefunction \( \Psi_{JM} \) of total orbital angular momentum \( J \) is expanded in terms of the Jacobi coordinates \( r_i \) and \( R_i \), \( (\alpha \) numbers the three rearrangement channels) as

\[ \Psi_{JM} = \sum_{\alpha} \sum_{i=1}^3 \sum_{J_{\alpha} L_{\alpha} I_{\alpha}} \sum_{i=1}^3 \sum_{I_{\alpha}} C_{\alpha J_{\alpha} L_{\alpha} I_{\alpha} i} \Phi_{\alpha J_{\alpha} L_{\alpha} I_{\alpha} i}, \]

(38)

\[ \Phi_{\alpha J_{\alpha} L_{\alpha} I_{\alpha} i} = N_{\alpha J_{\alpha} L_{\alpha} I_{\alpha} i} R_i^\alpha e^{-\mu/\alpha_0^2} e^{-(R_i/R_{\alpha 0})^2} \]

\[ [Y_{\alpha J_{\alpha}} (\mathbf{R}_\alpha) \otimes Y_{\alpha I_{\alpha}} (\mathbf{R}_\alpha)]_{JM}. \]

(39)

Here \( I_{\alpha} \) and \( L_{\alpha} \) are the angular momenta along \( r_i \) and \( \mathbf{R}_\alpha \), respectively, \( i \) and \( I \) are numbers of Gaussians along the two radial coordinates. The angular momenta \( I_{\alpha} \) and \( L_{\alpha} \) are chosen consistent with the total \( J \) i.e. \( |I_{\alpha} - L_{\alpha}| \leq J \leq I_{\alpha} + L_{\alpha} \), up to some maximum values \( I_{\alpha \text{max}} \) and \( L_{\alpha \text{max}} \), which may be different for different rearrangement channels.

For \( S \)-waves we used orbital angular momenta \( I_{\alpha} = L_{\alpha} \) from 0 to 4 in all three rearrangement channels. This gives a total of 15 configurations. For \( P \) and \( D \)-waves the total number of configurations used was 24. Typically a total of about 8000 Gaussians was used.
has been employed to determine the energies $E_{d_{1},\nu}$ and widths $\Gamma_{d_{1},\nu}$. That is, the binding energy $\varepsilon_{d_{1},\nu}$ becomes complex for resonances, $\varepsilon_{d_{1},\nu} = E_{d_{1},\nu} - \xi_{n} - i\Gamma_{d_{1},\nu}/2$. For resonances in the dipole series, both the real and the imaginary part of the energy is expected to follow the scaling condition (20). The theoretical aspects of this method have been discussed in our previous publications and will not be repeated [20, 22, 29–31].

### 4.1. Polarisability

As derived above, the dominating long-range interaction between the ionic core and Ps is the dipole interaction $\sim 1/r^2$. Considering the long-range interaction between a single charged particle (electron or positron) and the ionic core, the leading correction to the Coulomb interaction will be the long-range part of the polarisation potential $\sim -\alpha_d/2r^4$ where $\alpha_d$ is a dipole polarisability. This potential is attractive for both the electron and the positron.

When we evaluate the polarisability potential of Ps interacting with the ionic core, we have to allow for the fact that when the electron and positron coalesce their combined charge is zero, and hence the polarisability should vanish in this situation. We have allowed this by, in addition to the polarisability terms

$$V_{\text{pol}}(r_{1/2}) = -\frac{\alpha_d}{2r_{1/2}^3}U(r_{1/2}),$$

also introducing a correction

$$V_{\text{corr}}(r_{1/2}, \rho) = \frac{\alpha_d}{\rho^3}U(\rho)e^{-r_{1/2}^2/\rho^2}. \quad (41)$$

Here $U(x) = (1 - e^{-x^2})^2$ is a cut-off function, ensuring that the potentials do not diverge at short distances. When $r = 0$ we have $r_1 = r_2 = \rho$ and the sum

$$V_{\text{pol}}(r_1) + V_{\text{pol}}(r_2) + V_{\text{corr}}(0, \rho) = 0,$$  

thus giving the desired cancellation. We have performed calculations with and without the polarisability terms, and with and without the correction $V_{\text{corr}}$. In general, we find negligible changes to the Ps-type resonances (as can be expected since the leading interaction is $\sim 1/r^2$). However, for the bound ground-state (when it exists), the influence is larger. In table 1 we compare our results for the $e^+\,-\,$Na and $e^+\,-\,$Li ground state to other results in the literature. (Here we tuned $r_e$ in (41) to 3 for Na and 6 for Li to get the best agreement with Han et al [25]. Since we have a free parameter in the model interaction, our results are not variational, and could very well be lower than the true ground-state energy.)

### 5. Results and discussion

In table 2 we show the convergence using different sizes of the basis set for a typical resonance in the dipole series for $e^+\,-\,$Li system. We estimate the uncertainty to be in the resonance energy is less than $10^{-6}$, and in the width less than $10^{-5}$.

The result using 5100 basis functions is clearly not converged, but the results using larger basis sets show good convergence. These results are well fitted by the function $a + b/N$ (where $N$ is the number of basis function). Extrapolating to an infinite basis the exact result should then be given by $a$ (provided that our basis functions are chosen in such a way that they properly explore the entire Hilbert space). From our fit we get $a = -0.080622$ and thus conclude that our results with 8000 basis functions is accurate with an uncertainty of about $10^{-5}$. The width does not show a clear trend, but all values lie well within $10^{-5}$, which we estimate as our uncertainty.

In table 3 we present the energy positions and widths of resonances in the $e^+\,$H and $e^+\,-\,$A systems below the Ps ($n = 2$) threshold for $S$-, $P$-, and $D$-waves. Similar results have been published before so we defer detailed discussions.

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| Method            | without pol. | with pol. | with pol. + correction |
|-------------------|--------------|-----------|------------------------|
| $e^+\,-\,$Na      |              |           |                        |
| This work         | -0.250312    | -0.250710 | -0.250476              |
| AHM [39]          | ...          | ...       | -0.250447              |
| FCSVM [21]        | ...          | ...       | -0.250473              |
| FEM-ITM [40]      | ...          | ...       | -0.250357              |
| $e^+\,-\,$Li      |              |           |                        |
| This work         | -0.252386    | ...       | -0.252444              |
| AHM [39]          | ...          | ...       | -0.252455              |
| FCSVM [21]        | ...          | ...       | -0.252478              |
| FEM [41]          | ...          | ...       | -0.25237               |

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Table 1. Ground state energy of the $e^+\,-\,$Na and $e^+\,-\,$Li systems calculated using different models. The results are compared to the result of Han et al [39] using the same model potential as us, but with an additional term analogous to a ‘di-electronic correction’ added to the $e^+\,\,-\,e^-$ interaction to cancel the core polarisation when the two particles coalesce.

Table 2. Study of the rate of convergence for the different basis functions below the Ps ($n = 2$) state for the $e^+\,-\,$Li system. The notation $x[y]$ means $x \times 10^{-y}$. 

| No. of basis functions | $E_{21,\nu}$ | $\Gamma_{21,\nu}$ |
|------------------------|--------------|------------------|
| 5100                   | -0.08061620  | 2.20(4)          |
| 6050                   | -0.08062141  | 2.19(4)          |
| 6900                   | -0.08062156  | 2.22(4)          |
| 7500                   | -0.08062170  | 2.20(4)          |
| 8000                   | -0.08062182  | 2.18(4)          |
to these papers [20, 22, 29–31], though in some cases the present results have been extended and improved. (In particular, more resonances have been discovered for H, and D-wave calculations performed for K and Li.) Only very few resonances in these dipole series have been reported before. We compare to previous results in table 4.

Using these numerical results we obtain the scaling of successive dipole-state energies and widths as in table 5. We find for the most part excellent convergence to the expected analytical scaling law as the threshold is approached, especially for the energies. For the widths, which are more difficult to calculate accurately, the agreement is less good but still convincing. The more deeply bound states deviate more, as can be expected since the scaling law is exact only in the limit $\varepsilon \rightarrow 0$. There are also some other aberrations; the P-wave resonance located at $E_{21,0} = -0.06367517$ in H, as well as the resonances at $-0.06428345$ in Li and $-0.06306132$ in Na, do not seem to fit into the dipole sequence and have been omitted in table 5. Their presence seems to somewhat affect the binding energies of the neighbouring states, pushing them apart as compared to the ideal scaling. For K, we did not find this type of resonance.

We also note that the widths of the more deeply bound resonances in the alkali systems do not seem to conform to the scaling relation, while the energy positions agree quite well. This could, of course, be due to numerical errors, but the relatively good agreement closer to a threshold (except for P-waves) indicates that there may be some other reason.

A possible reason is that the threshold opens between resonances 1 and 2 in the dipole series for Li and Na (Li(3s) has the energy $-0.07422$, Na(4s) has energy $-0.071585$). Similarly, the K(5s) state has energy $-0.063632$, and lies between the S- and P-wave resonances 2 and 3 and D-wave resonances 1 and 2. Since the opening of a new atomic threshold adds another possible decay channel for the resonance it is natural that this should have a significant impact on the width, while the energy position may be much less affected.

Inverting (19) we can now extract the non-universal parameter $\Lambda_0$ for the different atoms

$$\Lambda_0 = \sqrt{-2M\alpha e^{-\varepsilon/\alpha} e^{\pi\varphi/\alpha}}. \quad (43)$$

Because of the scaling symmetry of the dipole series, this parameter is defined uniquely only up to a factor $e^{i\pi/\alpha} = 1.9$.

The results are shown in table 6. The parameter $\Lambda_0$ is complex because $\varepsilon$ is, though in two cases we haven’t been able to determine the imaginary part. We find that for the unscreened Coulomb potential with $Z = 1$, $\Lambda_0 = 0.78$. For the alkalis, this value changes by at most 25%. For a given threshold (i.e. for the same $\alpha$ and $\varphi$) larger $\Lambda_0$ corresponds to a more deeply bound dipole series.

The results for the S- and P-waves are quite similar, while the D-wave differs. This can be understood. S-wave resonances arise from coupling of the configurations $\{Ps(2s), L = 0\}$ and $\{Ps(2p), L = 1\}$, while P-wave resonances arise from coupling of the configurations $\{Ps(2s), L = 1\}$ and $\{Ps(2p), L = 0\}$. If the angular momentum barrier...
Table 4. Comparison to the previous literature values for $S_\nu$, $P_\nu$, and $D$-wave $\text{Ps}(n=2)$ dipole series of resonances in $e^{-}$-H and $e^{-}$-alkali systems. The notation $x[y]$ means $x \times 10^{-y}$.

|                  | Our results | Literature values | Reference |
|------------------|-------------|------------------|-----------|
|                  | $E_{2J,\nu}$ | $\Gamma_{2J,\nu}$ | $E_{2J,\nu}$ | $\Gamma_{2J,\nu}$ |
| $e^{-}$-H, S-wave |            |                  |           |           |
| $-0.07515883$    | $3.34[4]$   | $-0.075169$      | $3.12[4]$ | [19]       |
| $-0.06583801$    | $1.63[4]$   | $-0.065852$      | $1.62[4]$ | [42]       |
| $-0.06338973$    | $5.02[5]$   | $-0.063403$      | $5.04[5]$ | [42]       |
| $-0.06273766$    | $1.39[5]$   | $-0.062735$      | $1.58[5]$ | [42]       |
| $e^{-}$-Li, S-wave |            |                  |           |           |
| $-0.08062182$    | $2.18[4]$   | $-0.087525$      | $1.47[3]$ | [23]       |
| $-0.080685$      | $2.15[4]$   | $-0.086085$      | $2.02[4]$ | [43, 44]   |
| $-0.089436$      | $4.85[3]$   | $-0.086381$      | $6.9[5]$  | [25]       |
| $-0.06389506$    | $6.08[5]$   | $-0.064740$      | $4.85[3]$ | [27]       |
| $e^{-}$Na, S-wave |            |                  |           |           |
| $-0.07678850$    | $1.51[4]$   | $-0.07144$       | $7.3[6]$  | [23]       |
| $-0.075882$      | $4.3[4]$    | $-0.07680$       | $1.4[4]$  | [25]       |
| $-0.08155$       | $5.55[4]$   | $-0.08591$       | $3.1[4]$  | [24]       |
| $-0.06659598$    | $6.91[5]$   | $-0.06656$       | $6.1[5]$  | [25]       |
| $-0.06362215$    | $1.61[5]$   | $-0.06353$       | $4.1[5]$  | [25]       |
| $e^{-}$K, S-wave |            |                  |           |           |
| $-0.07284175$    | $1.38[4]$   | $-0.077415$      | $5.14[4]$ | [24]       |
| $-0.068227$      | $1.98[5]$   | $-0.068824$      | $1.98[5]$ | [23]       |
| $e^{-}$H, P-wave |            |                  |           |           |
| $-0.07408897$    | $3.02[4]$   | $-0.074091$      | $2.96[4]$ | [17]       |
| $-0.06537106$    | $1.51[4]$   | $-0.065365$      | $1.64[4]$ | [17]       |
| $-0.06367517$    | $7.00[5]$   | $-0.063676$      | $6.88[5]$ | [17]       |
| $e^{-}$Li, P-wave |            |                  |           |           |
| $-0.07894557$    | $1.07[4]$   | $-0.083850$      | $4.78[3]$ | [23]       |
| $-0.087882$      | $5.5[3]$    | $-0.085320$      | $1.13[2]$ | [43, 44]   |
| $-0.06676122$    | $1.26[4]$   | $-0.06884$       | $5.5[3]$  | [43, 44]   |
| $-0.068562$      | $1.62[3]$   | $-0.068562$      | $1.62[3]$ | [27]       |
| $e^{-}$Na, P-wave |            |                  |           |           |
| $-0.07518531$    | $1.00[4]$   | $-0.07405$       | $1.2[3]$  | [23]       |
| $-0.07787$       | $3.36[3]$   | $-0.07787$       | $3.36[3]$ | [28]       |
| $e^{-}$H, D-wave |            |                  |           |           |
| $-0.07194258$    | $1.69[4]$   | $-0.071965$      | $1.68[4]$ | [45]       |
| $-0.06446984$    | $6.90[5]$   | $-0.064475$      | $6.96[5]$ | [45]       |
| $e^{-}$Li, D-wave |            |                  |           |           |
| $-0.07595458$    | $1.40[4]$   | $-0.07260$       | $2.9[4]$  | [27]       |
| $-0.06532603$    | $4.36[5]$   | $-0.06841$       | $7.3[4]$  | [27]       |
| $e^{-}$Na, D-wave |            |                  |           |           |
| $-0.07259891$    | $4.96[4]$   | $-0.07126$       | $1.10[3]$ | [23]       |
| $-0.07313$       | $6.44[3]$   | $-0.07313$       | $6.44[3]$ | [28]       |

Ps$(n = 2)$ threshold $E_\nu = (-0.062500$ a.u.)

Table 5. Energy and width ratios of successive resonances located by the present calculation for $\text{Ps}(n = 2)$.

|                      | Present results | Analytical value |
|----------------------|-----------------|------------------|
| $e^{-}$-H            | $3.79$          | $3.58$          |
| $e^{-}$-Li           | $3.75$          | $3.62$          |
| $e^{-}$-Na           | $3.74$          | $3.71$          |
| $e^{-}$-K            | $3.73$          | $3.73$          |

$L(L+1)/(2M\mu^2)$ has only a limited influence on the short-range part of the wavefunction, the radial functions $f_{200,\nu}(\rho)$ and $f_{201,\nu}(\rho)$, would be rather similar, which could explain why $\Lambda_0$ is similar. (Note, that in the short-range part we cannot picture the problem just as a $\text{Ps}$ interacting with a core, since the atomic configuration $A+e^{-}$ may dominate.) The D-wave resonances on the other hand arise from coupling of three configurations, $\{\text{Ps}(2s), L = 2\}$, $\{\text{Ps}(2p), L = 1\}$, and $\{\text{Ps}(2p), L = 3\}$ and is therefore likely to be quite different.
We further note that the scaling relations seem to work reasonably well down to binding of at least 0.0015, which is well within our estimate $\varepsilon \ll 2^{-3/2} = 0.3$. For H and S-waves the scaling formula predicts the next lower resonance at $-0.1097$, corresponding to $\varepsilon = -0.047$. Though our calculations have exposed another resonance below the dipole series, its calculated energy $-0.128687$, or $\varepsilon = -0.066$ [20] does not fit well into the series. Again, another threshold $H(n = 2)$ at $-0.125$ may disturb the series. For Na the next lower resonance in the series would have the projected energy $-0.1158$, close to the $3p$ threshold $-0.1115$. We have not found such a resonance in our calculations, though other works have reported a resonance, which perhaps could be a candidate [23–25, 28]. However, in some of the works this resonance was found just above the $3p$ threshold, and we argued that in this case, it may have been a misidentified continuum state [20]. Similar conclusions hold for Li [31]. For K finally, we do find a candidate resonance at $-0.1031095$ ($\varepsilon = -0.0406095$) [30], while the energy predicted from the dipole scaling would be $-0.1011$ ($\varepsilon = -0.0388$), which perhaps also could be interpreted as part of the dipole series.

An interesting feature of the alkali-$e^+$ systems is that some form a stable ground state (Li,Na), while others do not (K). This ground state lies below the Ps(1s) threshold $-0.25$. We find that the systems which do support a bound state have larger $\Lambda_0$ at Ps(n = 2) (energy $-0.0625$), and the more deeply bound Li has the largest $\Lambda_0$. The heaviest alkali, K, which doest not have a bound $e^+$-K state has $\Lambda_0$ slightly smaller than H. Though the energy separation between the threshold is too large to draw any conclusions, this could perhaps be indicative of a similar short-range physics at both energies, yielding more attraction for Li and Na than for K.

### Table 6. The non-universal $\Lambda_0$ properties of $e^+$-H and $e^+$-alkali systems below the Ps(n = 2).

|                  | $e^+$-H | $e^+$-Li | $e^+$-Na | $e^+$-K |
|------------------|---------|---------|---------|---------|
| **S-wave**       | 0.78 − 0.023i | 0.98 − 0.018i | 0.87 − 0.0063i | 0.71 − 0.015i |
| **P-wave**       | 0.82 − 0.020i | 0.99 − 0.019i | 0.88 | 0.72 |
| **D-wave**       | 0.21 − 0.005i | 0.26 − 0.0030i | 0.22 − 0.0063 | 0.18 − 0.0013 |

6. Conclusion

In summary, we find that the analytical analysis of the dipole series in Ps-A$^+$ systems (or equivalently $e^+$-A systems) has a large predictive power. Due to the favourable mass scalings, many dipole resonances are predicted to exist within the energy range where the theory is valid. The formalism can also be extended to predict scattering properties.

We also find that complex scaling as applied to the coupled-rearrangement-channel method is a very powerful tool to calculate these resonances. For S-, P- and D-waves we have been able to numerically predict about 7 resonances in each Ps(n = 2) series, for all atoms investigated. For the most part, excellent agreement between numerical results and the analytical theory was obtained. However, in some cases, disagreements appeared which could be due to the proximity of atomic states, which were not included in the analytical analysis.

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### References

[1] Efimov V N 1970 Phys. Lett. B 33 563
[2] Efimov V N 1970 Yad. Fiz. 12 1080
[3] Efimov V N 1979 Yad. Fiz. 29 1058
[4] Efimov V N 1979 Sov. J. Nucl. Phys. 29 546
[5] Kraemer T et al 2006 Nature 440 315
[6] Zaccanti M, Deissler B, D’Errico C, Fattori M, Jona-Lasinio M, Müller S, Roati G, Inguscio M and Modugno G 2009 Nat. Phys. 5 586
[7] Knoop S, Ferlaino F, Mark M, Berninger M, Schöbel H, Nägerl H-C and Grimm R 2009 Nat. Phys. 5 227
[8] Berninger M, Zenesini A, Huang B, Harm W, Nägerl H C, Ferlaino F, Grimm R, Julienne P S and Hutson J M 2011 Phys. Rev. Lett. 107 120401
[9] Braaten E and Hammer H-W 2006 Phys. Rep. 428 259
[10] von Stecher J, D’Incao J P and Greene C H 2009 Nat. Phys. 5 417
[11] Temkin A and Walker J F 1965 Phys. Rev. 140 A1520
[12] Mittleman M H 1966 Phys. Rev. 152 76
[13] Ho Y K and Greene C H 1987 Phys. Rev. A 35 3169
[14] Ho Y K 1988 Phys. Lett. A 133 43
[15] Gien T T 1996 J. Phys. B: At. Mol. Opt. Phys. 29 2127
[16] Zhou Y and Lin C D 1995 J. Phys. B: At. Mol. Opt. Phys. 28 4907
[17] Ho Y K and Yan Z C 2004 Phys. Rev. A 70 032716
[18] Yan Z C and Ho Y K 2005 Phys. Rev. A 72 030701(R)
[19] Varga K, Mitroy J, Mezei J Z and Kruppa A T 2008 Phys. Rev. A 77 044502
[20] Umair and Jonsell S 2014 J. Phys. B: At. Mol. Opt. Phys. 47 225001
[21] Mitroy J, Bromley M W J and Ryzhik G G 2002 J. Phys. B: At. Mol. Opt. Phys. 35 R81
[22] Umair M and Jonsell S 2015 Phys. Rev. A 92 012706
[23] Ward S J, Horbatsch M, McEachran R P and Stauffer A D 1989 J. Phys. B: At. Mol. Opt. Phys. 22 3763
[24] Kar S and Ho Y K 2005 Eur. Phys. J. D 35 453
[25] Han H, Zhong Z, Zhang X and Shi T 2008 Phys. Rev. A 77 012721
[26] Han H, Zhong Z, Zhang X and Shi T 2008 Phys. Rev. A 78 044701
[27] Liu F, Cheng Y, Zhou Y and Jiao L 2011 Phys. Rev. A 83 032718
[28] Jiao L, Zhou Y, Cheng Y and Yu R M 2012 Eur. Phys. J. D 66 48
[29] Umair M and Jonsell S 2015 J. Phys.: Conf. Ser. 635 082001
[30] Umair M and Jonsell S 2016 J. Phys. B: At. Mol. Opt. Phys. 49 015004
[31] Umair M and Jonsell S 2016 Phys. Rev. A 93 052707
[32] Varshalovich D A, Moskalev A N and Khersonskii V K 1988 Quantum Theory of Angular Momentum (Singapore: World Scientific) p 291
[33] Kamimura M 1988 Phys. Rev. A 38 621
[34] Hiyama E, Kino Y and Kamimura M 2003 Prog. Part. Nucl. Phys. 51 223
[35] Ho Y K 1983 Phys. Rep. 99 1
[36] Reinhardt W P 1982 Ann. Rev. Phys. Chem. 33 223
[37] Junker B R 1982 Adv. At. Mol. Phys. 18 208
[38] Moiseyev N 1998 Phys. Rep. 302 212
[39] Han H, Li Y, Zhang X and Shi T 2008 J. Chem. Phys. 128 244314
[40] Shertzer J and Ward S J 2010 Phys. Rev. A 81 064505
[41] Shertzer J and Ward S J 2006 Phys. Rev. A 73 022504
[42] Zhou Y and Lin C D 1995 J. Phys. B: At. Mol. Phys. 28 4907
[43] Roy U and Ho Y K 2002 J. Phys. B: At. Mol. Opt. Phys. 35 2149
[44] Roy U and Ho Nucl Y K 2004 Nucl. Instrum. Methods Phys Res. B 221 36
[45] Yan Z C and Ho Y K 2002 J. Phys. B: At. Mol. Phys. 35 1875