Zero energy resonances in atomic processes within a plasma

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Abstract. We investigate different atomic processes that might occur in the interior of plasmas. In particular we apply the Final-State Interaction theory in order to study the behavior of the corresponding cross sections when the relative energy of a pair of charged particles in the initial or final states vanishes. Through this analysis we uncover the presence of zero-energy resonances for particular configurations of density and temperature. For fusion plasmas, these effects might have an important impact on the working conditions and performance of the reactor.

1. Introduction
Let us consider an atomic transition taking place within a plasma [1]. Naturally, the corresponding transition matrix element $T$ depends on the parameters that characterize the atomic partners before or after the transition. Furthermore, it also depends on the given conditions of density and temperature of the plasma, since they can affect the corresponding interactions. A well-known example is given by the screening length $\lambda$ of the interaction between charged particles.

In many cases of interest, the situation where the relative momentum $k$ of a pair of charged partners in the initial or final configuration vanishes can be relevant for the transition under study. When $k\lambda \gg 1$, the screened potential amplitudes converge to those for a pure Coulomb interaction, but this condition should fail for small enough values of $k$.

In this article we discuss on very general grounds the kind of consequence that such a screening might have on the atomic transitions taking place within the plasma, and whether they might be observable or lead to sizeable effects.

2. Final State Interaction Theory
According to the Final-State Interaction (FSI) theory [2, 3], the $k \to 0$ limit of $T$ is dominated by the inverse of the $s$-wave Jost function $f_0(k, \lambda)$ [4] (Atomic Units are used throughout this article, except where otherwise stated)

$$f_0(k, \lambda) = 1 + \frac{2m}{k} \int_0^\infty e^{ik\lambda}V_\lambda(r) \phi_{0k}(r) \, dr.$$ (1)

Here $V_\lambda(r)$ is the screened Coulomb potential between the active particles of reduced mass $m$ and relative momentum $k$ and distance $r$, while $\phi_{0k}(r)$ represents the $\ell = 0$ regular solution of
the radial equation. For small values of \( k\lambda \), this wave function becomes linear in \( k \), and therefore

\[
f_0(k, \lambda) \propto \frac{1 - ika}{a},
\]

where \( a \) is the scattering length for the potential \( V_{\lambda}(r) \).

For a pure Coulomb interaction \( V(r) = -Z/r \), i.e. for \( \lambda \to \infty \), we obtain

\[
f_0(k, \infty) = \frac{e^{-\pi\mu/2}}{\Gamma(1 - i\mu)},
\]

with \( \mu = mZ/k \) the so-called Gamow factor. Here we are considering only attractive (i.e. \( Z > 0 \)) potentials, since they are the ones that -as it is shown in this article- are prone to produce the larger distortions of the transition \( T \)-matrix elements through zero-energy resonances. The case of repulsive potentials (\( Z < 0 \)) can be readily obtained \textit{mutatis mutandis} from the present results.

When factored out of the \( T \)-matrix element for small values of \( k \), \( f_0(k, \lambda) \) would produce an enhancement factor \( F(k, \lambda) = \frac{1}{|f_0(k, \lambda)|^2} \), with very different behaviors for screened or unscreened potentials. For finite values of \( \lambda \), we obtain,

\[
F(k, \lambda) \propto a^2 \frac{1}{1 + k^2 a^2} \quad \text{for} \quad k \ll 1/\lambda,
\]

while for a pure Coulomb potential \( \lambda = \infty \),

\[
F(k, \infty) \approx \frac{2\pi mZ}{k} \quad \text{for} \quad k \ll mZ.
\]

We clearly see that the two limits \( k \to 0 \) and \( \lambda \to \infty \) do not commute [5, 6]. This behavior is similar to the one observed on the half-energy shells for the Coulomb off-energy-shell transition matrix element [7, 8, 9, 10].

One of the most striking effects produced by this diverging enhancement factor [11] is the Electron Capture to the Continuum (ECC) peak that can be observed in the momentum distribution of electrons emitted in atomic collisions when the velocity of the electron matches that of the projectile, i.e., when the relative electron-projectile momentum \( k \) vanishes. This effect was observed for outgoing ions [12, 13] and neutral atoms [14, 15, 16]. More recently, a similar effect was observed in positron-atom ionization collisions [17, 18].

3. Hulthèn potential

As a working example of the general theory sketched in the previous section, let us consider the Hulthèn potential

\[
V^H_{\lambda} = -\frac{Z}{\lambda} \frac{e^{-r/\lambda}}{1 - e^{-r/\lambda}}.
\]

The \( s \)-wave Jost function can be analytically evaluated for this exponentially screened Coulomb potential [5],

\[
f_0(k, \lambda) = \frac{\Gamma(1 - 2i k \lambda)}{\Gamma(1 + i\beta) \Gamma(1 - i\beta - 2i k \lambda)}
\]

with

\[
\beta = k \lambda \left[ \left( 1 - \frac{2\mu}{k \lambda} \right)^{1/2} - 1 \right].
\]
Except for a logarithmic distortion of the phase, we recover the pure Coulomb case for $k\lambda \gg 2\mu$ 
\[f_0(k, \lambda) = f_0(k, \infty) e^{-i\mu \ln(2k\lambda)}.\] 
(9)

On the other hand, for $k\lambda \ll 2\mu$,
\[\mathcal{F}(k, \lambda) = \frac{2mZ}{\lambda} \frac{a^2}{1 + k^2a^2},\] 
(10)

with
\[a = \frac{\pi \lambda}{\sin(\pi \sqrt{2mZ\lambda})}.\] 
(11)

We see that this enhancement factor would produce a Lorentzian-shape peak with a width or the order of $1/a$. However, the scattering length becomes infinite whenever $\mu$.
\[\lambda = \frac{n^2}{2mZ} \quad \text{with} \quad n = 1, 2, 3, \ldots\] 
(12)

At these zero energy resonances, the enhancement factor diverges like $k^{-2}$, and is responsible for the observation of the ECC effect even by neutral outgoing projectiles [14, 15, 16]. Any of these behaviors are extremely different from the $k^{-1}$ divergence produced by a pure Coulomb potential. These results are not unique to the Hulthén potential, but are generally valid for any exponentially screened or cut-off Coulomb potential [6]. Hence, we variationally adjust the charge $Z$ in order to correctly match the spectral properties of the Jost function for the Hulthén potential to those corresponding to a Yukawa potential. The analysis of the energy spectrum of the bound $s$–states [19] suggests to change $Z \to \alpha Z$ with $\alpha \approx 0.58$.

4. Radiative Recombination Processes

In order to illustrate the kind of effects that a zero-energy resonance might produce on an atomic process within a plasma, let us apply the previous results to a simple radiative recombination process, where an electron is captured by an ion into a $1s$ bound state with emission of a photon. For any given value of $\lambda$, we variationally adapt the typical radius of the final hydrogenic $1s$ state to reproduce a Yukawa $s$–state and, according to the FSI theory, incorporate on the cross section $\sigma$ the effects of the screening on the initial continuum state by means of the enhancement factor $\mathcal{F}(k, \lambda) = 1/|f_0(k, \lambda)|^2$. We observe that for the particular case of a Hulthén potential, the values of $\lambda$ at which the zero energy resonances occur, as given in Eq. (12), are in agreement with those obtained in recent numerical calculations of photoionization of hydrogen and hydrogen-like helium [20, 21] that employ a Debye screening potential within the framework of the complex-coordinate rotation method. For instance, the resonances observed in Figs. 1 and 2 of Ref. [20] and in Figs. 2 and 4 of Ref. [21] match those of Eq. 12 for $n = 2$. Even the successive resonances evaluated in Ref. [21] for He and He$^+$ with an exponential-cosine-screened Coulomb potential verify the $Z^{-1}$ and $n^2$ scaling rules predicted by Eq. 12. These results substantiate the validity of our simple and general approach. Furthermore, they seem to indicate that the observed resonances might correspond to zero-energy effects and not to shape-resonances resulting from quasi-bound $np$ states, as stated in Ref. [21].

As we have already mentioned, the screening length $\lambda$ depends on the plasma temperature $T$ and the particle density $\rho$ of the plasma electrons. For a static limit of the ion velocity, we can relate them in a very simple way by means of the standard interpolation [22, 23], which in atomic units reads,
\[\lambda^2 \approx \frac{1}{4\pi \rho} \left( T + \frac{(3\pi^2 \rho)^{2/3}}{3} \right).\] 
(13)
For simplicity, we consider a static limit, where the ion velocity is assumed to be much lower than the electron thermal velocity. Then, the reaction frequency can be calculated from

\[ \nu = \rho \langle \sigma v \rangle = \rho \int d^3 k f(k) \sigma(k) k , \]

where \( f(k) \) is the distribution function of the plasma electrons. We use a Maxwellian distribution function which is valid for high temperature plasmas [24], and \( \sigma \) is the total cross section for the radiative recombination process [25].

**Figure 1.** Reaction frequency for the radiative recombination of H\(^+\) and He\(^{2+}\) in a dense plasma as those used in inertial confinement fusion (with \( \rho = 10^{25}\) cm\(^{-3}\)) as a function of the temperature \( T \). A Hulthén potential was employed to model the screened electron-nucleus interaction. The index \( n \) characterizes the zero energy resonances, as described in the text.

In Fig. 1 we show the reaction frequency for the radiative recombination of H\(^+\) and He\(^{2+}\) in the case of inertial confinement (with \( \rho = 10^{25}\) cm\(^{-3}\)) as a function of the temperature \( T \) of the plasma. As described in the previous sections, a Hulthén potential was employed to model the screened electron-nucleus interaction. We clearly observe that the averaging on the momentum \( k \) of the plasma electrons is not enough to wash out the zero-energy resonances. Actually, the reaction frequency increases by as much as an order of magnitude or even more whenever the temperature \( T \) matches the zero energy resonance condition given by Eq. (12).

5. Conclusions
In this article we have uncovered the presence of zero energy resonances in plasmas for particular configurations of density and temperature. We applied our model to the particular case of a
radiative recombination process, but the same effects will be present in any atomic process, as for instance photoionization or electron-impact ionization, whenever the relative momentum of a pair of charged partners in the initial or final configuration vanishes. The relevance that these resonances might have on the working conditions and performance of a fusion reactor for inertial or magnetic confinement is to be analyzed and pondered.

Acknowledgments
This work was supported by the Comisión Nacional de Energía Atómica, CNEA (Controlled Nuclear Fusion Program) and Universidad Nacional de Cuyo (Grant 06/C416). ROB is also member of the Consejo Nacional de Investigaciones Científicas y Técnicas (CONICET), Argentina. CFC acknowledges the support of CONICET.

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