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2012 J. Phys.: Conf. Ser. 388 152034

(http://iopscience.iop.org/1742-6596/388/15/152034)

Feshbach-like study of He resonant states in Debye plasmas using explicitly correlated wave functions.

J. C. Cardona[1], **A. F. Ordoñez and J. L. Sanz-Vicario**[2]

Grupo de Física Atómica y Molecular. Instituto de Física, Universidad de Antioquia, Medellín, Colombia.

Synopsis We present a study on the $^{1,3}S^e$, $^{1,3}P^o$ and $^{1,3}D^e$ He resonant states below the He$^+$ (N=2) threshold under the influence of a plasma environment, when the Debye screening length is varied. The interaction between all charged particles is modeled with Yukawa-like screened Coulomb potentials. We make use of the Feshbach projector method to characterize resonant states, implemented by using explicitly correlated CI-wave functions.

Atomic processes occurring in a plasma environment have gain a raising interest during the last few years. Theoretical results are of interest not only in atomic physics but also in astrophysics, chemical physics, few-body physics and, of course, plasma physics. In this work, we study the behavior of resonance parameters (energies and lifetimes) of the lowest series of $^{1,3}S^e$, $^{1,3}P^o$ and $^{1,3}D^e$ He-like doubly excited states (optically accessed by one- or two-photon absorption) located below the N=2 ionization threshold, when the Debye characteristic length is varied. The non relativistic Hamiltonian for a two-electron system immersed into a weakly coupled plasma reads:

$$\mathcal{H} = -\frac{\nabla_1^2}{2} - \frac{\nabla_2^2}{2} - \frac{Z\exp(-r_1/D)}{r_1} - \frac{Z\exp(-r_2/D)}{r_2} + \frac{\exp(-r_{12}/D)}{r_{12}}, \quad (1)$$

where D=$(k_BT/4\pi e^2\rho)$ is the Debye length (a function of the plasma electron temperature T and density ρ) and it characterizes the strength of the interaction of the atomic system with the surrounding plasma. In this work we use a Hylleraas configuration interaction (HyCI) method to compute accurate energies and wave functions, the latter consisting of antisymmetrized correlated configurations $\psi_i(\mathbf{x}_1,\mathbf{x}_2)$=$\mathcal{A}\{\phi(\mathbf{r}_1,\mathbf{r}_2)\chi(s_1,s_2)\}$ where the spatial part of the wave function is built in terms of correlated Slater type orbitals:

$$\phi = r_1^{n_1} r_2^{n_2} r_{12}^{n_{12}} \mathrm{e}^{-\alpha r_1 - \beta r_2} \mathcal{Y}_{L,M}(\Omega_1,\Omega_2). \quad (2)$$

All integrals required for the solution of the plasma free (D=∞) as well as for finite values of D may be calculated in closed form [1, 2]. Previous extensive work by Ho *et al* (for instance [3, 4] and references therein) on atomic systems embedded in Debye plasmas makes use of the stabilization method to uncover resonances, which involves a demanding *many-diagonalizations* procedure. At variance, we have implemented a Feshbach projector operator method, which provides a rigorous procedure to split the resonant wave function into two orthogonal half-spaces. The square integrable resonant part $\mathcal{Q}\psi$ and the scattering-like part $\mathcal{P}\psi$. For two electron systems, the $\mathcal{P}$ projector is $\mathcal{P}$=$\mathcal{P}(1)$+$\mathcal{P}(2)$-$\mathcal{P}(1)\mathcal{P}(2)$ where $\mathcal{P}$(i)=$|\varphi_{1s}^D(i)\rangle\langle\varphi_{1s}^D(i)|$ must be constructed from Debye screened 1s orbitals. In our Feshbach-like implementation, the $(\mathcal{QHQ} - \epsilon_r)\mathcal{Q}\psi$=0 eigenvalue problem is replaced by its equivalent one $(\mathcal{H} + \mathcal{MP} - \epsilon_r)\psi$=0, where $\mathcal{MP}$ represents a Phillips-Kleinman pseudopotential. $\mathcal{P}$ space continuum wave functions are evaluated with uncorrelated configurations within a static exchange approximation. Resonant positions ϵ_r^D (plus shift corrections) and widths Γ^D are then readily calculated and systematic correlation diagrams (ϵ_r^D, Γ^D) vs. D shed light on the stability of doubly excited states embedded in a variety of plasma conditions and it also allows for a comparison with other available data.

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[1] E-mail: jcardona@fisica.udea.edu.co
[2] E-mail: sanjose@fisica.udea.edu.co