The photoionization of excited hydrogen atom in plasmas

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A B S T R A C T

The photoionization processes of excited hydrogen atoms in plasma environments are investigated using the method of complex coordinate rotation. The standard Debye–Hückel model and modified Debye–Hückel potentials, Debye–Hückel (DH) and modified Debye–Hückel (MDH) potentials, are adopted to describe the plasma screening effects. The photoionization cross sections of plasma-embedded excited hydrogen atoms varied with different screening lengths are displayed to illustrate the influence of plasma screening. The results of the Debye–Hückel model compared with the modified Debye–Hückel are presented. The shape resonances and Cooper minima due to the plasma screening are observed and discussed.

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1. Introduction

The plasma screening effects on photoionization have drawn increasing attention, since the photoionization is extremely sensitive to the details of atomic structure and electronic correlation effects. In recent years, there has been considerable effort devoted to the investigations of atomic photoionization spectrum in plasmas [1–4]. In this work, the method of complex coordinate rotation is adopted to study the influence of plasma screening on photoionization processes of excited hydrogen atoms due to the Debye–Hückel (DH) and modified Debye–Hückel (MDH) potentials,

\[
V(r) = \begin{cases} 
-\frac{1}{2} \exp(-r/\lambda_D) & \text{for DH,} \\
\frac{1}{2} \exp(-r/\lambda_D) \cos(r/\lambda_D) & \text{for MDH,}
\end{cases}
\]

where \( \lambda_D \) is the Debye screening length. The DH model is valid for weakly coupled plasmas, while the MDH model, in which electrons are treated as Fermi gas, is proposed by Shukla and Eliasson [5] to characterize the dense quantum plasmas. In the MDH model, the quantum statistical Fermi-pressure has been ignored, while the electron quantum force due to the quantum Bohm potential [6] is involved.

The plasmas are characterized by the parameters [7] related to temperature \( T \) and density \( \rho \). Quantum effects start to play an important role when the thermal de Broglie wavelength \( \lambda_B \) of the particles in plasmas is comparable to or larger than the interdistance \( \rho^{-1/3} \) of particles. Since the ratio \( \chi \equiv T_B/T \), where \( T_B \) is the Fermi temperature, is proportional to \( (\rho \lambda_B^3)^{3/2} \), \( \chi \ll 1 \) and \( \chi \gg 1 \) correspond to the classical and quantum case, respectively. The coupling parameter \( \Gamma \) defined by the ratio of the interaction energy to the average kinetic energy determines the plasma to be collisional (\( \Gamma \geq 1 \)) or collisionless (\( \Gamma \ll 1 \)). According to the definition, one can obtain \( \Gamma_C \sim \rho^{1/3}/T \) for classical cases, whereas \( \Gamma_D \sim \rho^{-1/3} \) for quantum cases. Based on a classical and collisionless framework, the DH model properly describes the classical plasma within the high temperature and low density regime. For the high density and low temperature regime, quantum effects, such as quantum-statistical and quantum-diffraction effects, become significant. The MDH model, in which the quantum force due to the Bohm potential acting on the electrons is provided to dominate over the Fermi pressure [5], takes the quantum-diffraction effect into account, but neglects the relatively small quantum-statistical effect.

On the other hand, the non-existence of Cooper minimum [8–10] or shape resonances for any states of free hydrogen atoms is well known. The shape resonances, however, induced by plasma screening effects are reported by the recent work on the ground-state photoionization of plasma-embedded H atoms and He\(^+\) ions [4]. In addition, the Cooper minima and shape resonances of hydrogen-like ions caused by the DH potential are also predicted by Qi et al. [11]. Therefore, the appearance of Cooper minima and shape resonances of hydrogen-like ions is highly expected for excited hydrogen atoms in plasmas, particularly the plasmas characterized by MDH potentials. The main purpose of this work is to comprehensively study the plasma screening effects of the MDH model and illustrate the different influence of the DH and MDH models on the photoionization processes. The comparison of the shielding effects due to these two models on photoionization cross sections of excited hydrogen atoms is displayed. The emphasis is placed on the shape resonances and Cooper minima occurring in cross section curves.
for photoionization from the 2s and 3s excited states of hydrogen atoms.

### 2. Theoretical methods

The theoretical method applied to the calculations of photoionization cross sections for the present work is based on the rigorous approach of complex coordinate rotation developed by Rescigno and McKoy [12]. The theoretical perspectives and applications of this method to atomic and molecular systems have been reviewed and discussed in articles by Reinhardt [13,14] and Ho [15] respectively. In addition, the discussion of crucial features of resonance wave functions and electronic density can be found in the review paper by Buchleitner et al. [16]. This method has been widely and successfully employed to study the atomic processes in strong electric field [17] and plasma environments [18,19]. In the present paper, only brief description of the method is given.

Based on the first order approximation, the Schrödinger equation for an atom in the presence of an electric field becomes [20]

\[(H - E_0 \pm \omega)\psi^\pm = \mu \psi_0,\]  

(2)

where \(\psi_0\) and \(E_0\) the wave function and energy of a stationary state for a target atom, \(\omega\) the photon energy, and \(\mu = \hat{e} \times r\) the dipole-length operator along the direction \(\hat{e}\) of the polarization of light. The negative frequency solution \(\psi^-\) is associated with the photoabsorption process. With the \(\psi^-\) obtained by Eq. (2), the negative frequency component of the polarizability is given by [12]

\[\alpha^-(\omega) = \langle \psi_0 | \mu | \psi^- \rangle, \]  

(3)

Within the framework of complex coordinate rotation approach, the transformation of radial coordinates, \(r \to r\Theta\) with \(\Theta = \exp(i\theta)\), are carried out, while the negative frequency wave functions \(\psi^-\) are expanded in terms of all optically allowed states \(\psi_i\). Eq. (3) becomes

\[\alpha^-_\theta (\omega) = \sum I \int d^3r \psi^\dagger_0 (r\Theta) \mu(r\Theta) \psi_i (r) \int d^3r \psi^\dagger_i (r) \mu(r\Theta) \psi_0 (r\Theta) \int d^3r \psi^\dagger_i (r) \mu(r\Theta) \psi_0 (r\Theta) \]  

(4)

In the present calculations, the wave function \(\psi_0(r\Theta)\) is obtained by an unrotated Hamiltonian and then transformed into complex coordinates of the radial variable, while the wave functions \(\psi_i(r)\) consisting of linear combinations of real discrete basis functions (unrotated basis functions) with complex coefficients are acquired from a rotated Hamiltonian. The eigenvalues \(E_i\) corresponding to \(\psi_i\) are complex. Note that the conjugate functions \(\psi^\dagger_0\) and \(\psi^\dagger_i\) are defined by taking the complex conjugate of angular part only, but not of radial part.

Utilizing the optical theorem, the photoionization cross sections in the electric dipole approximation are given by

\[\sigma(\omega) = \frac{4\pi \omega}{c} \text{Im}(\alpha^-_\theta (\omega)), \]  

(5)

where \(c\) the speed of light, i.e., the inverse fine-structure constant.

### 3. Results and discussion

The 2s-, 3s-, and 4s-state photoionization cross sections of hydrogen atoms in DH plasmas are given in Fig. 1. For either case, the ionization thresholds are shifted toward lower photon energies with decreasing the Debye screening lengths. In Fig. 2, the comparisons of cross section results obtained by the MDH model to results by the DH model are displayed. For the same Debye screening lengths \(\lambda_0\) (in units of \(a_0\)).
lengths, the lower ionization thresholds of the MDH model indicate the greater screening of the MDH model than the DH model.

The extra cosine factor in the MDH potential produces the oscillatory behavior in the long range part of the potential curve. As a result, the sign change due to the cosine factor results in the less attractive potential and meanwhile creates repulsive potential barriers as compared to the DH potential. It leads to the lower ionization thresholds of the MDH model than the DH model for the same Debye screening length, and explains the greater screening effect in the MDH model.

The photoionization cross sections for the 2s excited state of hydrogen in the MDH model varied with a wide range of Debye screening lengths are presented in Fig. 3. There are three groups of resonances appearing for certain ranges of Debye screening lengths, particularly for the Debye screening lengths of 6.73, 14.45, and 25.2 which give the sharpest peak of the resonances. In Fig. 4, the cross sections of the 2s excited state are given as functions of photoelectron energies, in which all ionization thresholds associated with different plasma screening are normalized to the zero photoelectron energy. The comparisons of three groups of resonances in Fig. 4 show the existence of Cooper minima accompanied by the first group of resonances with the Debye screening lengths between 6.5 and 6.73.

The energies for hydrogen atom in several excited states varied with Debye screening lengths are displayed in Fig. 5. The ns and np states, which are degenerate for the free hydrogen case, are gradually
Fig. 5. Energies of the modified Debye–Hückel model as functions of Debye screening lengths $\lambda_D$ for the 2s–4s (dashed lines) and 2p–4p (solid lines) excited states. The numbers indicated in the figure are the critical Debye screening lengths for each state.

Fig. 6. Systematic variation of the 3s-state photoionization cross sections with a wide range of Debye screening lengths $\lambda_D$ (in units of $a_0$) indicated in the figure for the modified Debye–Hückel model.

ally splitting and moving toward the thresholds with the decrease of Debye screening lengths. The $ns$ and $np$ bound states will turn into continua as the Debye screening lengths are less than the critical values, which are indicated in Fig. 5 for each bound state. The critical Debye screening lengths of the MDH model for the 2p, 3p, and 4p states are 6.75, 14.56, and 25.47 respectively, which correspond to the three groups of resonances in Fig. 3. When the Debye screening lengths are slightly less than one of these critical values, the bound state being shifted toward the continuum causes a quasi-bound state supported by the centrifugal barrier of potentials and gives rise to the shape resonance.

In Fig. 6, the systematic variation of cross sections with a wide range of Debye screening lengths for hydrogen atoms in the 3s excited state is given. The comparisons of resonance profiles associated with the 3p, 4p, and 5p quasi-bound states are presented in Fig. 7. For the 3s-state photoionization, only the shape resonances associated with the 3p quasi-bound state accompany the emergence of Cooper minima in the cross section curves.

4. Conclusions

The photoionization processes of excited hydrogen atoms in plasmas characterized by the DH and MDH potentials have been studied using the method of complex coordinate rotation. Comparing the results of the DH model to the MDH model shows...
that plasma screening effects significantly alter the profile of cross sections for photon energies near the ionization thresholds. The bound states are shifted toward the ionization thresholds with decreasing the Debye screening lengths. When the Debye screening lengths are less than and near the critical Debye screening lengths, the quasi-bound states caused by bound states turning into the continua but captured by the centrifugal barrier of potentials prominently enhance the cross sections. Besides the shape resonances, the plasma-induced Cooper minima also have been observed for excited hydrogen atoms. For 2s- and 3s-state photoionization, only shape resonances associated with 2p and 3p quasi-bound state respectively can be accompanied by the appearance of Cooper minima.

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