## Frequency-dependent stabilization of He<sup>-</sup> by a superintense laser field

Qi Wei and Sabre Kais

Department of Chemistry, Purdue University, West Lafayette, Indiana 47907, USA

Nimrod Moiseyev

Department of Chemistry and the Minerva Center for Non-Linear Physics of Complex Systems, Technion, Haifa 32000, Israel (Received 21 May 2007; published 17 July 2007)

Using the alternative representation of time-dependent Hamiltonians that describe laser-driven systems [I. Gilary and N. Moiseyev, Phys. Rev. A **66**, 063415 (2002)], we have performed calculations for the stability of He<sup>-</sup> in a superintense linearly polarized laser field. We estimated the laser parameters, amplitude, and frequency needed to stabilize He<sup>-</sup>. If we choose the laser frequency  $\omega=5$  eV, the laser intensity needed for stabilization is  $I^{\text{critical}}=9.0 \times 10^{15}$  W/cm<sup>2</sup> and the maximal detachment energy is 1.0 eV. Our results show that high frequencies and large intensities are preferred for stabilizing multiply negative atomic ions in superintense laser fields.

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Atomic stabilization by superintense lasers is of fundamental importance in atomic and molecular physics and has attracted considerable theoretical attention over the past two decades [1-10]. The idea that negative charged atomic ions can be stabilized and the photoinduced ionization can be suppressed in the presence of a strong laser field has been proposed a long time ago (see Ref. [1], and references therein). However, due to the numerical complexity of the problem, stabilization calculations, where the electronic correlation is in the presence of the strong field, have been carried out only within the framework of the dressed picture formalism. Under this approximation, the time-independent many-electron effective potential depends on the  $\alpha_0$  $=eE_0/(m_e\omega^2)$  parameter, where  $E_0$  is the maximum field amplitude and  $\omega$  is the laser frequency. Therefore, these types of calculations can provide the desired information on the dependence of the stabilization of the anion on the two laser parameters,  $E_0$  and  $\omega$ . Using a representation of timedependent Hamiltonians of driven systems in strong laser fields enables us to go beyond the Kramers-Henneberger (KH) zero-order dressed potential [11]. By carrying out a transformation to obtain a time-averaged potential with a better dependence on the field's parameter [12] it has been shown that cold atoms can be trapped due to the quantum analog of the Kapitza mechanism where a classical particle is trapped by introducing an external rapid time periodic potential [13,14]. The purpose of this paper is to apply this approach to He<sup>-</sup> and to find out the laser parameters for which the photoinduced ionization is suppressed.

A monochromatic field of electric field vector has the following form:

$$\mathbf{E}(t) = E_0(\mathbf{e}_1 \cos \omega t + \mathbf{e}_2 \tan \delta \sin \omega t), \tag{1}$$

with  $\mathbf{e}_j$  (j=1,2) unit vectors orthogonal to each other and to the propagation direction,  $\delta=0$  corresponds to linear polarization and  $\delta=\pm \pi/4$  corresponds to circular polarization. The high-frequency Floquet theory that proceeds from the space translated version of the time-dependent Schrödinger equation for *N*-electron atoms reads as follows [1]:  $\sum_{i=1}^{N} \left[ \frac{1}{2} \mathbf{P}_{i}^{2} - \frac{Z}{|\mathbf{r}_{i} + \alpha(t)|} + \sum_{j=1}^{i-1} \frac{1}{|\mathbf{r}_{i} - \mathbf{r}_{j}|} \right] \Psi = i \frac{\partial \Psi}{\partial t}, \quad (2)$ 

where  $\alpha(t) = \frac{\alpha_0}{E_0} \mathbf{E}(t)$  with  $\frac{\alpha_0}{E_0} = 1/(m_e \omega^2)$ . This equation refers to a coordinate frame translated by  $\alpha(t)$  with respect to the laboratory frame. By using the Floquet ansatz one seeks to determine solutions to the following structure equation [1]:

$$\sum_{i=1}^{N} \left[ \frac{1}{2} \mathbf{P}_i^2 + V_0(\mathbf{r}_i, \alpha_0) + \sum_{j=1}^{i-1} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|} \right] \Phi = \varepsilon(\alpha_0) \Phi. \quad (3)$$

The Hamiltonian here contains the original Coulomb potential modified (dressed) by the laser field,  $V_0$ , which is referred to as the "dressed" potential. All of the eigenstates obtained from Eq. (3) are called the "dressed" states.

Here the dressed potential  $V_0$  is the time average of  $\frac{-Z}{|\mathbf{r}+\alpha(t)|}$ ,

$$V_0(\mathbf{r},\alpha_0) = -\frac{Z}{2\pi} \int_0^{2\pi} \frac{d\xi}{|\mathbf{r} + \alpha(\xi/\omega)|}.$$
 (4)

For linear polarization, the dressed potential  $V_0$  is equivalent to that of a linear charge with a relative larger charge density near the two endpoints and a smaller one near the center. The length of the linear charge is  $2\alpha_0$ . In a two-center coordinate system,  $V_0$  has the following form [15]:

$$V_0(\alpha_0, \mathbf{r}) = -\frac{2Z}{\pi} (\mathbf{r}_A \cdot \mathbf{r}_B)^{-1/2} K \left[ \left( \frac{1 - \hat{\mathbf{r}}_A \cdot \hat{\mathbf{r}}_B}{2} \right)^{1/2} \right], \quad (5)$$

where *A* and *B* are the two foci of the system (two endpoints of the linear charge). *Z* is the nuclear charge. *K* is the elliptical integral of the first kind. Recently, using Eq. (3), we calculated the laser critical parameters needed for the stability of He<sup>-</sup>, He<sup>2-</sup>, and Li<sup>2-</sup> in the linearly polarized superintense laser field [15]. The detachment energies depend on the laser parameter  $\alpha_0$  and the maximal values are 1.2, 0.12, and 0.13 eV, respectively [15].

In this paper, we use the representation of time-dependent theory, which was developed by Gilary and Moiseyev [12],



FIG. 1. (Color online) Negative detachment energy for He<sup>-</sup> in the linearly polarized (along the *z* axis) superintense laser field as a function of  $\alpha_0$  with different frequencies.

to describe the laser-driven atomic system. Unlike the highfrequency Floquet theory where the dressed potential depends on the characteristic parameter  $\alpha_0 = \sqrt{I}/\omega^2$ , where  $\omega$ and *I* are the laser frequency and intensity, this approach provides a time-average potential that depends explicitly on both of the field parameters, *I* and  $\omega$ . The modified equation is given by [12]

$$\sum_{i=1}^{N} \left[ \frac{1}{2} \mathbf{P}_{i}^{2} + V_{0}(\mathbf{r}_{i}, \alpha_{0}) + \frac{1}{2\omega^{2}} \sum_{n \neq 0} \frac{f_{n}(\mathbf{r}_{i})f_{-n}(\mathbf{r}_{i})}{n^{2}} + \sum_{j=1}^{i-1} \frac{1}{|\mathbf{r}_{i} - \mathbf{r}_{j}|} \right] \times \Phi = \varepsilon(\alpha_{0}, \omega) \Phi.$$
(6)

Here  $V_0$ , the dressed Coulomb potential, is from Eq. (4) and  $f_n(\mathbf{r})$  has the following form:

$$f_n(\mathbf{r}) = -\frac{\partial V_n(\mathbf{r})}{\partial z},\tag{7}$$

where

$$V_n(\mathbf{r}) = \frac{Z}{2\pi} \int_0^{2\pi} \frac{e^{-in\xi} d\xi}{|\mathbf{r} + \alpha(\xi/\omega)|}.$$
 (8)

For linear polarization it is convenient to use a two-center coordinate basis set of elliptical functions to perform the calculations. The basis has the following form [15]:

$$\Phi(\xi,\eta,\phi)_{p,q,m} = (\xi-1)^p \eta^q [(1-\eta^2)(\xi^2-1)]^{m/2} e^{-\gamma\xi} e^{im\phi},$$
(9)

where *p*, *q*, and *m* are non-negative integers, and  $\gamma$  is a variational parameter which will be used to optimize the numerical results.  $\xi$ ,  $\eta$ , and  $\phi$  are prolate spheroidal coordinates with  $\xi = \frac{r_A + r_B}{2\alpha_0}$  and  $\eta = \frac{r_A - r_B}{2\alpha_0}$ . Now we can proceed by using the self-consistent-field

Now we can proceed by using the self-consistent-field method to obtain the ground-state energy and wave function of a given atom with a nuclear charge Z in a laser field. Then we find the critical value of  $\alpha_0$  for binding N electrons to such a given atom. As long as  $\varepsilon^{(N)}(\alpha_0) > \varepsilon^{(N-1)}(\alpha_0)$ , one of the electrons on the N-electron ion autodetaches and therefore the atomic multiply charged negative ions are unstable. In order to determine the stability of an atomic multiply charged negative ion, we define  $\alpha_0^{\text{critical}}$  for which the detachment energy is  $D^{(N)}(\alpha_0^{\text{critical}})=0$ . The detachment en-

TABLE I. Critical parameters for the stability of He<sup>-</sup> in superintense laser fields using different approximate potentials.  $V_0$  is the well-known dressed potential and  $V_{\text{total}}$  is the new frequencydependent potential. The intensity is determined by the following equation:  $I=E_0^2/(2\mu_0c_0)$ , where  $E_0=m_e\alpha_0\omega^2/e$ ; here we choose  $\omega$ =5 eV.

	$lpha_0^{ ext{critical}}$ (a.u.)	<i>I</i> <sup>critical</sup> (W/cm <sup>2</sup> )	$\alpha_0^{\max}$ (a.u.)	I <sup>max</sup> (W/cm <sup>2</sup> )	Detachment energy (eV)
$\overline{V_0}$	11	$4.8 \times 10^{15}$	26	$2.7 \times 10^{16}$	1.2
$V_{\rm Total}$	15	$9.0  imes 10^{15}$	31	$3.9 \times 10^{16}$	1.0

ergy is the energy required to detach one of the *N* electrons from an ion at a particular value of  $\alpha_0$ ,  $D^{(N)}(\alpha_0) = \varepsilon^{(N-1)}(\alpha_0) - \varepsilon^{(N)}(\alpha_0)$ . Therefore, we can find the critical value of  $\alpha_0$  for which  $D^{(N)}(\alpha_0^{\text{critical}})=0$ . For values of  $\alpha_0$  larger than the  $\alpha_0^{\text{critical}}$ , none of the *N* electrons will autodetach, and the *N*-electron atomic multiply charged negative ion supports a bound state. We use the self-consistent-field methods to obtain the ground-state energy and wave function of the He<sup>-</sup> ion in the laser field. Then, we find the detachment energy as the frequency is varied.

The detachment energy as a function of  $\alpha_0$  for He<sup>-</sup> with different frequencies is shown in Fig. 1. It turns out that the new potential makes a great difference from the original  $V_0$ when the  $\alpha_0$  is small. But when the  $\alpha_0 > 100$  a.u., there is almost no difference. We performed a calculation for three different frequencies, 3, 5, and 15 eV. It shows that the perturbation increased quickly when the frequency is decreased. All the critical parameters for the stability of He<sup>-</sup> are listed in Table I. Notice, for example, if an ultrahigh-power KrF laser ( $\omega$ =5 eV) is used, the peak intensity is  $I^{\text{critical}}$ =4.8×10<sup>15</sup> W/cm<sup>2</sup> using the high-frequency Floquet



FIG. 2. (Color online) Electronic charge distribution for He<sup>-</sup> in the linearly polarized (along the *z* axis) superintense laser field at the critical point. Upper panel,  $\alpha_0=11$  a.u. and  $\omega=\infty$ , using the high-frequency Floquet dressed potential. Lower panel,  $\alpha_0^{\text{critical}}=15$  a.u. and  $\omega=5$  eV, using the total potential which includes the frequency-dependent term.



FIG. 3.  $\alpha_0^{\text{critical}}$  as a function of  $\omega$  for He<sup>-</sup> in the linearly polarized superintense laser field. In the high-frequency Floquet theory  $\alpha_0^{\text{critical}} = 11$  a.u.

dressed potential. However, when one uses the total potential which includes the frequency-dependent term, we have  $I^{\text{critical}} = 9.0 \times 10^{15} \text{ W/cm}^2$ .

In Fig. 2, we compare the electronic charge distribution for He<sup>-</sup> in a linearly polarized (along the *z* axis) superintense laser field at the critical point  $\alpha_0=11$  a.u., using the highfrequency Floquet dressed potential with the one at  $\alpha_0=15$  a.u., and  $\omega=5$  eV using the total potential which includes the frequency-dependent term. Both have the same shape, there is no overlap of the orbitals, however the latter is more spread out than the first one. Figures 3 and 4 show the critical  $\alpha_0$  and the binding energy as a function of  $\omega$ .

In summary, singly charged negative atomic helium is unstable in the gas phase [16-18] and the lifetime is only

- For an overview of superintense high-frequency phenomena, treated with the high-frequency Floquet theory, see M. Gavrila, *Atoms in Super Intense Laser Fields* (Academic, New York, 1992), p. 435.
- [2] E. van Duijn, M. Gavrila, and H. G. Muller, Phys. Rev. Lett. 77, 3759 (1996).
- [3] N. Moiseyev and F. Weinhold, Phys. Rev. Lett. 78, 2100 (1997).
- [4] N. Moiseyev and L. S. Cederbaum, J. Phys. B 32, L279 (1999).
- [5] E. van Duijn, M. Gavrila, and H. G. Muller, Phys. Rev. Lett. 77, 3759 (1996).
- [6] N. J. van Druten, R. C. Constantinescu, J. M. Schins, H. Nieuwenhuize, and H. G. Muller, Phys. Rev. A 55, 622 (1997); M. P. de Boer, J. H. Hoogenraad, R. B. Vrijen, R. C. Constantinescu, L. D. Noordam, and H. G. Muller, *ibid.* 50, 4085 (1994).
- [7] I. Vorobeichik, R. Lefebvre, and N. Moiseyev, Europhys. Lett. 41, 111 (1998).
- [8] M. Pont, N. R. Walet, M. Gavrila, and C. W. McCurdy, Phys. Rev. Lett. 61, 939 (1988).



FIG. 4. Maximal detachment energy (binding energy) as a function of  $\omega$  for He<sup>-</sup> in the linearly polarized superintense laser field. The binding energy in the high-frequency Floquet theory is 0.044 a.u.

around  $10^{-4}$  s [19], but in our case it is bound and stable. Our calculations show that for realistic laser parameters, i.e., second harmonics of KrF laser with feasible intensity, singly negative charged helium atoms can be prepared.

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- [9] N. Moiseyev and L. S. Cederbaum, J. Phys. B **32**, L279 (1999).
- [10] J. H. Eberly and K. C. Kulander, Science 262, 1229 (1993).
- [11] H. A. Kramers, *Collected Scientific Papers* (North-Holland, Amsterdam, 1956); W. C. Henneberger, Phys. Rev. Lett. 21, 838 (1968).
- [12] I. Gilary and N. Moiseyev, Phys. Rev. A 66, 063415 (2002).
- [13] I. Gilary, N. Moiseyev, S. Rahav, and S. Fishman, J. Phys. A 36, L409 (2003).
- [14] S. Rahav, I. Gilary, and S. Fishman, Phys. Rev. Lett. 91, 110404 (2003); S. Rahav, I. Gilary, and S. Fishman, Phys. Rev. A 68, 013820 (2003).
- [15] Q. Wei, S. Kais, and N. Moiseyev, J. Chem. Phys. 124, 201108 (2006).
- [16] J. P. Neirotti, P. Serra, and S. Kais, Phys. Rev. Lett. 79, 3142 (1997).
- [17] P. Serra, J. P. Neirotti, and S. Kais, Phys. Rev. Lett. 80, 5293 (1998).
- [18] S. Kais and P. Serra, Adv. Chem. Phys. 125, 1 (2003).
- [19] U. V. Pedersen, M. Hyde, S. P. Moller, and T. Andersen, Phys. Rev. A 64, 012503 (2001).