Role of higher multipoles in field-induced continuum lowering in plasmas

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(Received 24 July 2000; revised manuscript received 12 January 2001; published 24 April 2001)

The latest development in calculations of a continuum lowering (CL) in plasmas is based on the employment of dicenter models of the plasma state. One such theory—a percolation theory—calculated the CL defined as an absolute value of energy at which an electron becomes bound to a macroscopic portion of plasma ions (a quasi-ionization). We derived *analytically* the value of the CL in the ionization channel, which was disregarded in the percolation theory: a quasimolecule, consisting of the two ion centers plus an electron, can become ionized in the true sense of the word before the electron would be shared by more than two ions. We derived the CL in this channel for an arbitrary ratio of charges of the two Coulomb centers, while the specific values of the CL in the percolation theory were obtained only for dicenters consisting of two identical ions. We produced our results within a purely classical approach, but proceeding from *first principles*. We also showed that whether the electron is bound primarily by the smaller or by the larger out of two positive charges makes a dramatic qualitative and quantitative difference for this ionization channel. This difference is revealed due to our allowance for all higher multipoles.

DOI: 10.1103/PhysRevE.63.057401 PACS number(s): 52.25.−b, 31.15.Pf, 33.70.−w

I. INTRODUCTION

Continuum lowering (CL) in plasmas was studied for 40 years; see, e.g., books/reviews [1–3] and references therein. The CL plays a key role in calculations of the equation of state, partition function, bound-free opacities, and other collisional atomic transitions in plasmas (see, e.g., [4,5] and references therein). The latest development is based on the employment of dicenter models of the plasma state [1,6–11]. These models are more advanced than previously used ion sphere models (referred to in [1–3]).

Specific calculations of the CL on the basis of a dicenter model were presented in [1,8] and called a ''percolation theory of the CL.'' The starting point of this theory is the observation that a bound electron is localized within the volume of a given ion as long as its binding energy is well below the lowest potential barrier that separates its ion from the neighboring ones. When the energy approaches this lowest potential barrier, the electron may tunnel out from the ionic potential well. When this happens, its wave function overlaps two or more ions. Electronic states of increasingly higher energy overlap greater and greater clusters of ions. Above some critical value of the electron energy, which is noticeably higher than the top of the potential barrier U_{top} separating the radiating ion from its nearest neighbor, one of the clusters percolates, that is, the wave function of an electron having this or higher energy overlaps a macroscopic portion of the plasma ions. When this occurs, the electron can be regarded as a negative-energy continuum electron.

Apart from a questionable boundary condition used in this model (which was criticized in [10]), there is a serious conceptual flaw in this model. Indeed, at some value of energy slightly higher than U_{top}, the quasimolecule, consisting of the two ion centers plus an electron, can become ionized in the true sense of the word before the electron would be shared by more than two ions. In other words, the electron belonging to the dicenter can go directly into a true (positive-energy) continuum bypassing the multistage process of being shared by more and more ions.

In the present paper, we study the ionization of a molecule consisting of two Coulomb centers (TCC) plus an electron and we derive *analytically* the value of the CL in this ionization channel for an *arbitrary ratio of charges* of the TCC. (We note that specific values of the CL in the percolation theory [1,8] were obtained only for dicenters consisting of two identical ions.) We proceed in a purely classical approach and derive our results *from first principles*. In particular, we show that whether the electron is bound primarily by the smaller or by the larger out of two positive charges makes a dramatic qualitative and quantitative difference for this ionization channel. Our treatment is similar to our previous papers [12,13], where we demonstrated that a paradigm, in which level crossings and charge exchange in plasmas were considered as inherently quantum phenomena, is generally incorrect and that these phenomena actually have classical roots.

II. CLASSICAL TCC PROBLEM

We consider a system, where the charge Z is at the origin and the Oz axis is directed to the charge Z', which is at $z=R$ (here and below, the atomic units $\hbar=e=m_e=1$ are used). The charges Z and Z' are stationary. For simplicity, we confine ourselves to circular orbits of the electron: the orbit, whose plane is perpendicular to Oz, has a radius ρ and its center is at the Oz axis at some point z such that $0\leqslant z\leqslant R$. For $z\ll R$ or $(R-z)\ll R$, circular orbits depict Stark states, corresponding classically to the zero projection of the Runge-Lenz vector [14] on the axis Oz and corresponding quantum mechanically to the zero electric quantum number $q\equiv n_1-n_2$, where n_1,n_2 are the parabolic quantum numbers [15]. (For example, for $z\ll R$, it would be a hydrogenlike ion of the nuclear charge Z perturbed by a fully stripped ion of the nuclear charge Z'.) The states corresponding to $q=0$ provide a reasonable ''middle ground'' (between the states of $q>0$ and the states of $q<0$) for studying the ionization and the CL caused by it. We define the following dimensionless quantities: $b\equiv Z'/Z$, $v\equiv\rho/R$, and $w\equiv z/R$.

From the condition of the equilibrium along the *Oz* axis, it is easy to express the equilibrium value of v as a function of w (see [13] for details):

$$v(w,b)=\frac{\{[w(1-w)^2]^{2/3}-b^{2/3}w^2\}^{1/2}}{\{b^{2/3}-[w/(1-w)]^{2/3}\}^{1/2}}. \tag{1}$$

For $b<1$, the equilibrium value of v exists for $0\leqslant w<b/(1+b)$ and for $1/(1+b^{1/2})\leqslant w\leqslant 1$. For $b>1$, the equilibrium value of v exists for $0\leqslant w\leqslant 1/(1+b^{1/2})$ and for $b/(1+b)<w\leqslant 1$. For $b=1$, the equilibrium value of v exists for the entire range of $0\leqslant w\leqslant 1$. Below, we refer to these intervals as the ''allowed ranges'' of w.

From the condition of the equilibrium in the orbital plane, it is easy to find the equilibrium values of the electron velocity $V(w,b)$, and thus the kinetic energy $K(w,b)$, the total energy $E(w,b)$, as well as the angular momentum projection $M(w,b)$ on the axis *Oz*. Particularly,

$$E(w,b)=(Z/R)e(w,b),$$

$$e(w,b)\equiv-[w(1-w)+v^2(w,b)/2]/\{(1-w)\times[w^2+v^2(w,b)]^{3/2}\}; \tag{2}$$

$$M(w,b)=(ZR)^{1/2}l(w,b),$$

$$l(w,b)\equiv v^2(w,b)/\{(1-w)^{1/2}[w^2+v^2(w,b)]^{3/4}\}. \tag{3}$$

We consider energy terms of the *same symmetry*. In the quantum TCC problem, ''terms of the same symmetry'' means terms of the same magnetic quantum number m [16–20]. Therefore, in our classical TCC problem, from now on we fix the angular momentum projection M and study the behavior of the classical energy at $M=\text{const}\geqslant 0$ (the results for M and $-M$ are physically the same). From Eq. (3), we obtain

$$R(w,b,M)=M^2/[Z\,l^2(w,b)], \tag{4}$$

so that $z(w,b,M)=wR(w,b,M)$ and $\rho(w,b,M)=v(w,b)R(w,b,M)$. For any $b>0$, for any w from the allowed ranges (controlled by the value of b), and for any $M\geqslant 0$, the internuclear distance R, the location of the orbital plane z, and the radius of the orbit ρ each have its individual unique equilibrium value given by the functions $R(w,b,M)$, $z(w,b,M)$, and $\rho(w,b,M)$, respectively. Then we substitute $R(w,b,M)$ in Eq. (2) and find

$$E(w,b,M)=(Z/M)^2l^2(w,b)e(w,b)\equiv(Z/M)^2\epsilon(w,b). \tag{5}$$

Thus, for any $b>0$ and $M\geqslant 0$, Eqs. (4) and (5) determine in a parametric form (via w) the dependence of the energy E on the internuclear distance R, i.e., the *classical energy terms*. Figure 1 shows the dependence of the scaled total energy $(M/Z)^2E$ on the scaled internuclear distance $(Z/M^2)R$ (both quantities are dimensionless) for $b=2$. The results are totally counterintuitive. There is more than one classical energy term, i.e., there are three terms of the same symmetry. Moreover, two of these classical energy terms undergo a V-shaped crossing.

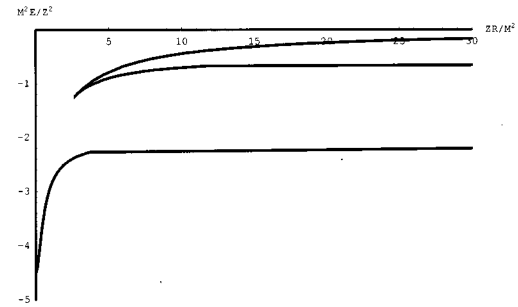

FIG. 1. Classical energy terms: the dependence of the scaled (dimensionless) total classical energy $(M/Z)^2E$ on the scaled (dimensionless) internuclear distance $(Z/M^2)R$ for $Z'=2Z$.

We emphasize that the above example of $Z'/Z=2$ represents a typical situation. In fact, for any pair of Z and $Z'\neq Z$ there are three classical energy terms of the same symmetry and the upper term always crosses the middle term. (For $Z'=Z$, there is only one term in the corresponding plot and no crossing, as should be expected.)

Our analysis showed [12,13] that these three energy terms have the following origin. At $R\to\infty$, the middle term translate into the energy E of the hydrogenlike ion of the nuclear charge $Z_{\min}\equiv\min(Z',Z)$, $[E\to-(Z_{\min}/M)^2/2]$, slightly perturbed by the charge $Z_{\max}\equiv\max(Z',Z)$. It corresponds to a classically *stable* motion. As for the upper term, at $R\to\infty$, it translates into a near-zero-energy state (where the electron is almost free). The classical motion, corresponding to the upper term, is *unstable*. Therefore, when the hydrogenlike ion of the nuclear charge $Z_{\min}$, being perturbed by the charge $Z_{\max}$, reaches a point, corresponding to the crossing of these two terms, the electron ''switches'' from the stable motion to the unstable motion. The radius of the electron orbit and the distances of the electron from both positive charges experience an unlimited increase, which is equivalent to the ionization of the molecule.

To avoid any confusion, we emphasize that our analysis presented in [13] was not limited to circular orbits of the electron. For clarity, we briefly outline here the scheme of our analysis. In the cylindrical coordinates (z,ρ,ϕ), using the axial symmetry of the problem, we separated the z and ρ motions from the ϕ motion. (Later on, the ϕ motion was determined from the obtained ρ motion.) Then we studied equilibrium points of the two-dimensional motion in the $z\rho$ space. We explicitly found the condition distinguishing between two physically different cases: (i) the effective potential energy has a two-dimensional minimum in the $z\rho$ space; (ii) the effective potential energy has a saddle point in the $z\rho$ space. In particular, it turned out that the boundary between these two cases corresponds to the point of crossing of the upper and middle energy terms.

III. ANALYSIS OF THE CONTINUUM LOWERING

Figure 2 shows the dependence of the scaled total energy $e(w,b)$, defined in Eq. (2), versus the dimensionless distance

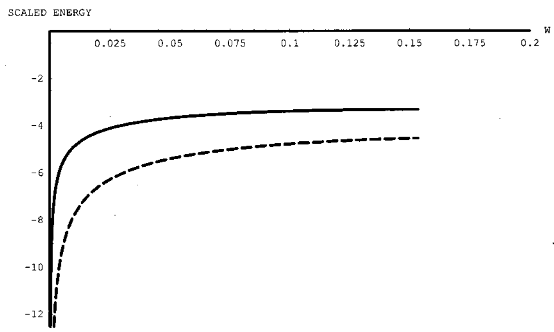

FIG. 2. A calculated dependence of the scaled (dimensionless) total classical energy $(R/Z)E(w,b)$, defined in Eq. (2), vs the dimensionless distance $w=z/R$ of the electronic orbital plane from the charge Z for $b=2$ (solid line). Only the branch of $(R/Z)E(w,b)$, corresponding to the middle energy term in Fig. 1, is shown in Fig. 2. The dashed line shows the dependence of the scaled potential energy $u(w,b)=(R/Z)U(w,b)$ vs w for $b=2$.

w of the electronic orbital plane from the charge Z for $b=2$. Only the branch of $e(w,b)$, corresponding to the middle energy term in Fig. 1, is shown in Fig. 2. The dashed line in Fig. 1 shows the dependence of the scaled potential energy $u(w,b)=(R/Z)U(w,b)$ versus w for $b=2$ [here $U(w,b)$ is the potential energy]. The crossing point between the middle (stable) and upper (unstable) terms in Fig. 1 corresponds to the maximum of the $e(w,b)$, i.e., to a value w_c where $\partial e/\partial w=0$. This is the point of a transition from a stable motion to an unstable motion, leading the electron to the zero energy (i.e., to the free motion) along the upper energy term in Fig. 1, which constitutes the ionization of the molecule.

We emphasize again that the above example of $Z'/Z=2$ represents a typical situation. In fact, for any pair of Z and $Z'\neq Z$, the transition from a stable to an unstable motion, followed by the ionization of the molecule, corresponds to the maximum of $e(w,b)$ versus w. At the point $w_c(b)$, where the maximum occurs, the scaled energy $e(w_c(b),b)$ differs from zero (it is negative). Thus, we arrive at the following. For the ionization of the hydrogenlike ion of the nuclear charge $Z_{\min}$ perturbed by the charge $Z_{\max}$, it is sufficient to reach the scaled energy $e(w_c(b),b)<0$. At that point, the electron switches to the unstable motion and the radius of its orbit increases without a limit. This constitutes a CL by the amount of $\Delta E=Z\langle 1/R\rangle|e(w_c(b),b)|$, where $\langle 1/R\rangle$ is the value of the inverse distance of the nearest-neighbor ion from the radiating ion averaged over the ensemble of perturbing ions.

Figure 3 shows the calculated dependence of the scaled (dimensionless) value of this CL $\Delta E/(Z\langle 1/R\rangle)$ versus Z'/Z (in the double-logarithmic scale). It is seen that the CL increases rather rapidly with the growth of Z'/Z, especially for Z'/Z in the range from 1 to 2. In the range of Z'/Z from 1 to 16, this dependence can be approximated (within an inaccuracy of less than 1%) as follows:

$$\Delta E/(Z\langle 1/R\rangle)\approx 1.800(Z'/Z)^{9.202}/[0.1691+(Z'/Z)^{8.327}]. \tag{6}$$

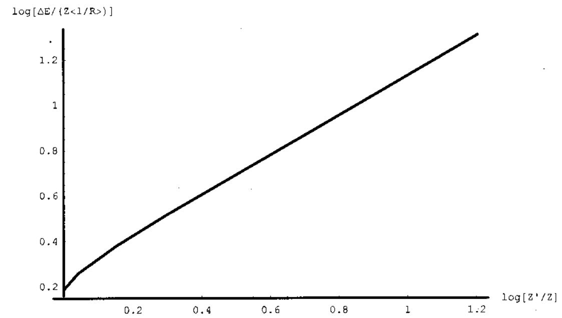

FIG. 3. A calculated dependence of the scaled (dimensionless) value of the continuum lowering $\Delta E/(Z\langle 1/R\rangle)$ on Z'/Z for a hydrogenlike ion of the nuclear charge $Z_{\min}\equiv\min(Z',Z)$, slightly perturbed by the charge $Z_{\max}\equiv\max(Z',Z)$. The plot is in the double-logarithmic scale, the base of the logarithms being 10.

We emphasize that our value of the CL is found with the allowance for all higher multipoles and therefore supersedes in accuracy any of the previously published classical results obtained while keeping only the dipole term or the dipole plus quadrupole terms.

Now we proceed to the lower-energy term (see Fig. 1). At $R\to\infty$, the lower term translates into the energy of the hydrogenlike ion of the nuclear charge $Z_{\max}$, $[E\to -(Z_{\max}/M)^2/2]$, slightly perturbed by the charge $Z_{\min}$. It corresponds to a *stable* classical motion. At $R\to 0$, the lower term translates into the energy of the hydrogenlike ion of the nuclear charge $Z+Z'$, $(E\to -[(Z+Z')/M]^2/2)$. It corresponds to a *stable* classical motion as well. The lower term does not cross any term, corresponding to an unstable motion.

This means that for the hydrogenlike ion of the nuclear charge $Z_{\max}$ perturbed by the charge $Z_{\min}$, the true (nonpercolational) ionization is impossible (in the classical approach). In other words, no matter how close the charge $Z_{\min}$ would be to the charge $Z_{\max}$ and how big would be the electric field, acting on the hydrogenlike ion due to the charge $Z_{\min}$, *no true ionization* would occur; the system would remain in a bound state of the molecule ZeZ'. (In this case, only the percolational process [1,8] leading to a quasi-ionization would be possible.) Thus, whether the electron is bound primarily by the smaller or by the larger out of two positive charges makes a dramatic qualitative and quantitative difference for the ionization channel we considered. We emphasize that the latter result cannot be obtained by going only one step beyond the dipole approximation and taking into account the quadrupole interaction. Only the allowance for all higher multipoles reveals a dramatic qualitative difference between the two cases discussed above.

IV. CONCLUSIONS

We derived *analytically* the value of the CL in the ionization channel, which was disregarded in the percolation theory [1,8] of the CL. We derived the CL for an arbitrary ratio of charges of the two Coulomb centers, while the specific values of the CL in the percolation theory [1,8] were obtained only for dicenters consisting of two identical ions.

We produced our results within a purely classical approach, but proceeding from *first principles*.

We believe that the importance of our results in two-fold. First, they should motivate quantum studies of the CL channel, which was missing in [1,8]. Second, we showed (for the first time, to the best of our knowledge) that whether the electron is bound primarily by the smaller or by the larger out of two positive charges makes a *dramatic qualitative and quantitative difference* for this CL channel. This difference is revealed due to our allowance for all higher multipoles.

Thus, plasmas having ions of different nuclear charges require further quantum studies of both the CL in the percolation theory and the CL discussed by us, as well as a subsequent comparison of the CL in these two channels. We note that plasmas having ions of different nuclear charges are quite common for a variety of applied projects. Some important examples are (i) laser fusion, where a thermonuclear fuel is a *D-T* mixture and/or where a low-*Z* thermonuclear fuel is doped by a high-*Z* material for diagnostic purposes; (ii) plasmas resulting from a laser interaction with composite solid targets (see, e.g., [21,22]); (iii) powerful *Z* pinches used as plasma radiation sources for various applications (see, e.g., [23]).

Finally, we note that we did not include the electron screening in any way. However, our classical description of the above problem, in principle, can be generalized by allowing for the Debye screening as well as by going beyond the circular states of the TCC problem. Such work is now in progress.

[1] D. Salzmann, *Atomic Physics in Hot Plasmas* (Oxford University Press, Oxford, 1998), Chaps. 2 and 3.

[2] M. S. Murillo and J. C. Weisheit, Phys. Rep. **302**, 1 (1998).

[3] H. R. Griem, *Principles of Plasma Spectroscopy* (Cambridge University Press, Cambridge, 1997), Secs. 5.5 and 7.3.

[4] C. Stehle, J. M. Caillol, A. Escarguel, and D. Gilles, J. Phys. IV **10**, Pr5-501 (2000).

[5] D'jachkov, J. Quant. Spectrosc. Radiat. Transf. **59**, 65 (1998).

[6] J. Stein, I. B. Goldberg, D. Shalitin, and D. Salzmann, Phys. Rev. A **39**, 2078 (1989).

[7] D. Salzmann, J. Stein, I. B. Goldberg, and R. H. Pratt, Phys. Rev. A **44**, 1270 (1991).

[8] J. Stein and D. Salzmann, Phys. Rev. A **45**, 3943 (1992).

[9] P. Malnoult, B. D'Etat, and H. Nguen, Phys. Rev. A **40**, 1983 (1989).

[10] Y. Furutani, K. Ohashi, M. Shimizu, and A. Fukuyama, J. Phys. Soc. Jpn. **62**, 3413 (1993).

[11] P. Sauvan, E. Leboucher-Dalimier, P. Angelo, H. Derfoul, T. Ceccotti, A. Poquerusse, A. Calisti, and B. Talin, J. Quant. Spectrosc. Radiat. Transf. **65**, 511 (2000).

[12] E. Oks, Phys. Rev. Lett. **85**, 2084 (2000).

[13] E. Oks, J. Phys. B **33**, 3319 (2000).

[14] L. D. Landau and E. M. Lifshitz, *Mechanics* (Pergamon, Oxford, 1960).

[15] L. D. Landau and E. M. Lifshitz, *Quantum Mechanics* (Pergamon, Oxford, 1965).

[16] S. S. Gershtein and V. D. Krivchenkov, Zh. Eksp. Teor. Fiz. **40**, 1491 (1961) [Sov. Phys. JETP **13**, 1044 (1961)].

[17] J. Von Neumann and E. Wigner, Phys. Z. **30**, 467 (1929).

[18] L. I. Ponomarev and T. P. Puzynina, Zh. Eksp. Teor. Fiz. **52**, 1273 (1967) [Sov. Phys. JETP **25**, 846 (1967)].

[19] J. D. Power, Philos. Trans. R. Soc. London, Ser. A **274**, 663 (1973).

[20] I. V. Komarov, L. I. Ponomarev, and S. Yu. Slavyanov, *Spheroidal and Coulomb Spheroidal Functions* (Nauka, Moscow, 1976) (in Russian).

[21] K. Eidmann, A. Saemann, U. Andiel, I. E. Golovkin, R. C. Mancini, E. Anderson, and E. Förster, J. Quant. Spectrosc. Radiat. Transf. **65**, 173 (2000).

[22] E. Leboucher-Dalimier, P. Angelo, T. Cecotti, H. Derfoul, A. Poquerusse, P. Sauvan, E. Oks, A. Calisti, and B. Talin, in *Inertial Fusion Science and Applications, Proceedings of the International Conference, Bordeaux, France, 1999* (Elsevier, Paris, 2000), p. 1115.

[23] J. P. Apruzese, J. W. Thornhill, K. G. Whitney, J. Davis, C. Deeney, T. J. Nash, R. B. Spielman, P. L'Eplattenier, P. D. LePell, B. H. Failor, J. C. Riordan, B. A. Whitton, E. J. Yadlowsky, R. C. Hazelton, and J. J. Moschella, IEEE Trans. Plasma Sci. **26**, 1185 (1998).