Single ionization of helium by electron impact

I. Bray, D. V. Fursa, A. S. Kadyrov, and A. T. Stelbovics
Australian Research Council Centre for Antimatter-Matter Studies, Curtin University of Technology, General Post Office Box U1987, Perth, Western Australia 6845, Australia
(Received 18 November 2009; published 8 June 2010)

We suggest that the problem of single ionization of helium by electron impact, leaving the ion in the ground state, has been solved theoretically for the full range of kinematics and collision geometries of practical interest. Following the emphasis on the study of out-of-plane geometries where the cross sections are very small [Schulz *et al.*, Nature **422**, 48 (2003)], we find that the convergent close-coupling calculations, in either a frozen- or a multicore treatment of the target, are in excellent agreement with the available measurements. Curiously, some systematic discrepancies are identified for some in-plane cases where the cross sections are an order of magnitude larger. Further measurements are required to resolve these discrepancies. If subsequent measurements confirm the present calculations, then we would have a strong case that the problem has been solved.

DOI: 10.1103/PhysRevA.81.062704 PACS number(s): 34.80.Dp

I. INTRODUCTION

Quantum collision physics is one of the most important fields in the study of the properties of matter. The understanding of collisions in atomic and molecular physics is required in a broad range of sciences and applications, including astrophysics, plasma physics, lighting, and many others. Such collisions are governed by the long-range Coulomb potential and so are also prototypes of collisions with more general and complicated potentials.

The electron-helium (e-He) scattering system is one of the most experimentally studied of all collision systems due to the relative ease of generating well-defined projectile and target beams in the laboratory. For the theorists, atomic hydrogen would be the preferred target, but the complexity of obtaining it in a laboratory has meant that considerably fewer experiments have been performed for atomic hydrogen than helium. Fortunately, due to the very strong binding of the 1s electron in He^+, the computational complexity of the e-He problem can be reduced substantially by allowing for only one electron excitation. The validity of such a treatment is readily checked by having a multicore (MC) description of the target.

The goal of complete approaches to calculating electron-atom collisions is to be able to accurately describe all of the dominant excitation and ionization processes irrespective of the incident energy, kinematics, or geometrical orientation of the outgoing electrons [1]. Only nonperturbative approaches to the problem are able to do so. The exterior complex scaling (ECS) method has been very successful in describing electron-impact ionization of atomic hydrogen [2,3], and this has been extended also to excitation [4,5]. The time-dependent close coupling (TDCC) and the convergent close coupling (CCC) also are in excellent agreement with the few available experiments involving atomic hydrogen [6,7] but additionally have been extensively applied to the helium target; see Colgan *et al.* [8] and references therein. The key question is whether there is sufficient agreement between the wide-ranging experimental data and theory to declare the e-He single ionization a solved problem.

Keeping in mind that agreement with experimental results can never prove a theory to be correct, yet a single discrepancy can invalidate it, it is very difficult to demonstrate a problem to have been solved. Historically, it is common for theoretical development to follow experimental observation. Perhaps the best we can hope for is for a theory to be predictive by preempting experimental observation or suggest that existing theory is sufficiently accurate and that a conflicting experiment deserves to be revisited.

When electrons collide with helium, the dominant cross section is elastic scattering. This is due to the fact that helium is an inert gas with very high excitation and ionization thresholds. Consequently, the excitation and ionization cross sections are relatively small and difficult to calculate accurately. Nevertheless, several approaches based on the close-coupling method such as the R matrix (see, e.g., [9,10] and references therein) and the CCC method [11] generally are in excellent agreement with experimental results. We emphasize that though the validity of computational methods generally depends on the projectile energy range, this is not the case with the CCC method, which was developed to be valid on the entire energy range of interest [12,13]. This is not only important when generating data for applications as a function of energy but also particularly helpful when trying to identify the source of discrepancies with experimental results.

We are confident that the e-He elastic scattering and excitation problems are solved in the sense that the CCC theory is able to yield accurate scattering amplitudes of the major discrete target states at all scattering energies [14,15]. The problem of ionization is more complicated. Though the underlying formal theory for the discrete transitions has been well developed for many decades, this is not the case for ionization. Only very recently has the definition of the post form of the ionization amplitude has been given that is suitable for computation [16,17]. Following this development, the success of the ECS and CCC approaches to ionization can now be understood, and we may pose the question as to whether the e-He single-ionization problem has also been computationally solved.

II. THEORY

The details of the CCC approach to ionization have been given by Bray and Fursa [18] and Stelbovics *et al.* [19]. Briefly, the target states ϕ_n with energies ε_n are obtained by

diagonalizing the target Hamiltonian in a complete Laguerre (square-integrable) basis of size N. With increasing N, the resulting negative-energy states converge to the true discrete target states, while the positive-energy states provide for an increasingly dense discretization of the target continuum. In the case of helium, the diagonalization involves two electrons. In the frozen-core (FC) treatment, one of the electrons is described by the $1s$ orbital of He^+. This works generally well for all of the excited states but causes the ionization energy of the ground state to be 23.74 eV rather than the experimental 24.59 eV. In such calculations, we reduce the incident energy by 0.85 eV to ensure the same total (excess) energy in the calculations as in the experiment of interest. By additionally allowing several short-ranged Laguerre functions for the "inner" electron, the MC calculations are able to be performed that yield an ionization energy within 0.1 eV of the true result. Unfortunately, such calculations yield many more states, all of which need to be included in the close-coupling expansion. Consequently, the MC calculations typically require considerably more computational resources.

Once the states are defined, they are used to expand the total wave function of the electron-target system, with the resulting close-coupling equations solved in momentum space. This yields transition amplitudes $T_{fi}^{(N)}(\boldsymbol{k}_f,\boldsymbol{k}_i)$ for excitation of the initial target state ϕ_i to ϕ_f by an initial electron of momentum $\boldsymbol{k}_i$ and final momentum $\boldsymbol{k}_f$. The total energy (a.u.) E of the system is $E = \varepsilon_f + k_f^2/2 = \varepsilon_i + k_i^2/2$.

For $\varepsilon_f < 0$, the $T_{fi}^{(N)}(\boldsymbol{k}_f,\boldsymbol{k}_i)$ are used directly to generate elastic scattering and excitation information for comparison with experimental results. We associate ionization processes with the $T_{fi}^{(N)}(\boldsymbol{k}_f,\boldsymbol{k}_i)$ for which $\varepsilon_f > 0$. These display a step-function behavior whereby $\lim_{N\to\infty} T_{fi}^{(N)}(\boldsymbol{k}_f,\boldsymbol{k}_i) = 0$ for $\varepsilon_f > E/2$ [20]. For finite N, the scattering amplitudes behave as Fourier expansions of step functions [21], with the physical ionization information contained in the $T_{fi}^{(N)}(\boldsymbol{k}_f,\boldsymbol{k}_i)$ for $0 < \varepsilon_f \leqslant E/2$. By interpolating the $T_{fi}^{(N)}(\boldsymbol{k}_f,\boldsymbol{k}_i)$, available at discrete values of ε_f, on to a continuous energy scale, we are able to define the ionization amplitudes $T_i^{(N)}(\boldsymbol{k}_1,\boldsymbol{k}_2,\boldsymbol{k}_i)$, where $\boldsymbol{k}_1 \equiv \boldsymbol{k}_f$ and $\boldsymbol{k}_2$ are constructed from the ϕ_f.

III. COMPARISON WITH EXPERIMENTAL RESULTS

There is an extraordinarily large amount of experimental data available for e-He (single) ionization for various kinematics and geometrical orientation of the detectors. Figure 1 shows a convenient way of parametrizing the ionization process. The two outgoing electrons of energies $e_1 = k_1^2/2$ and $e_2 = k_2^2/2$ form the scattering plane. The two scattering angles θ_1 and θ_2 are on the opposite sides of the dashed line, which is the projection of the incident beam onto the scattering plane. For the so-called symmetric geometries of interest to us presently, we have $\theta_1 = -\theta_2$. In such geometries, forward and backward angles correspond to both electrons being emitted in similar directions where the cross sections are generally very small.

In the coplanar case, the incident electron is also in the same plane, that is, $\psi = 0^\circ$, and such geometries typically have the largest cross sections. In the perpendicular plane geometries ($\psi = 90^\circ$), the cross sections are often particularly small.

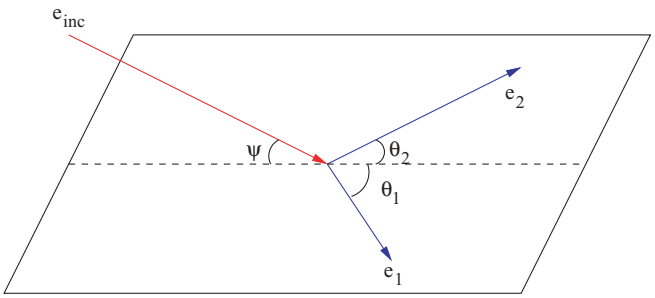

FIG. 1. (Color online) The parameters involved in electron-atom ionization. Here an incident electron of energy $e_{\rm inc}$ coming at angle ψ to the scattering plane with outgoing electrons of energies e_1 and e_2 at scattering angles θ_1 and θ_2.

Schulz *et al.* [22] considered the single ionization of helium by heavy projectile impact. The energies considered were so large that high-energy approximations were considered to be more than adequate for the complete description of the ionization process. However, while this was indeed the case for the large cross sections in the coplanar geometry, this was not so for the much smaller cross sections in the out-of-plane geometries. While this particular problem remains unresolved as far as we are aware [23], it certainly generated considerable interest in measuring and calculating e-He ionization in out-of-plane geometries [24,25]. The broad goal is to test the nonperturbative approaches to ionization against the smaller out-of-plane cross sections.

In Fig. 2, we present coplanar ($\psi = 0^\circ$) and perpendicular-plane ($\psi = 90^\circ$) fully differential cross sections for electron-impact ionization of helium with the specified electron energies of the outgoing electrons. Note that the $\theta_1 = 90^\circ$ is a common point to both geometries; see Fig. 1.

Beginning at the top for the lowest energies with $e_1 = e_2 = 1$ eV, corresponding to an incident electron of 26.6 eV, we see that both geometries yield almost identical cross sections in both shape and magnitude. Given the preference for back-to-back emission at low energies, it is interesting that the maximum cross section is when the incident beam is perpendicular to the outgoing electrons. This is in fact only a local maximum, with the maximal cross section being around three times bigger for back-to-back emission with the incident electron being parallel to one of the outgoing electrons [19]. Agreement of the CCC calculation with the coplanar absolute data of Rösel *et al.* [26] is excellent, and it would be helpful to have the perpendicular-plane theoretical prediction considered by a future experiment.

The next row has $e_1 = e_2 = 4$ eV, corresponding to an incident energy of 32.6 eV, and we see a substantial shape change of the coplanar cross section but not of the magnitude. However, the perpendicular plane shows only a slight narrowing in shape but a factor of two drop in magnitude. Again, agreement with the absolute experiment [27] is excellent, but it is only available for the coplanar case.

The $e_1 = e_2 = 10$ eV case, corresponding to an incident energy of 44.6 eV, is particularly interesting because we have two independent sets of measurements of the coplanar geometry reported by Murray *et al.* [28] and Rioual *et al.* [29], and a measurement of the perpendicular-plane geometry [28].

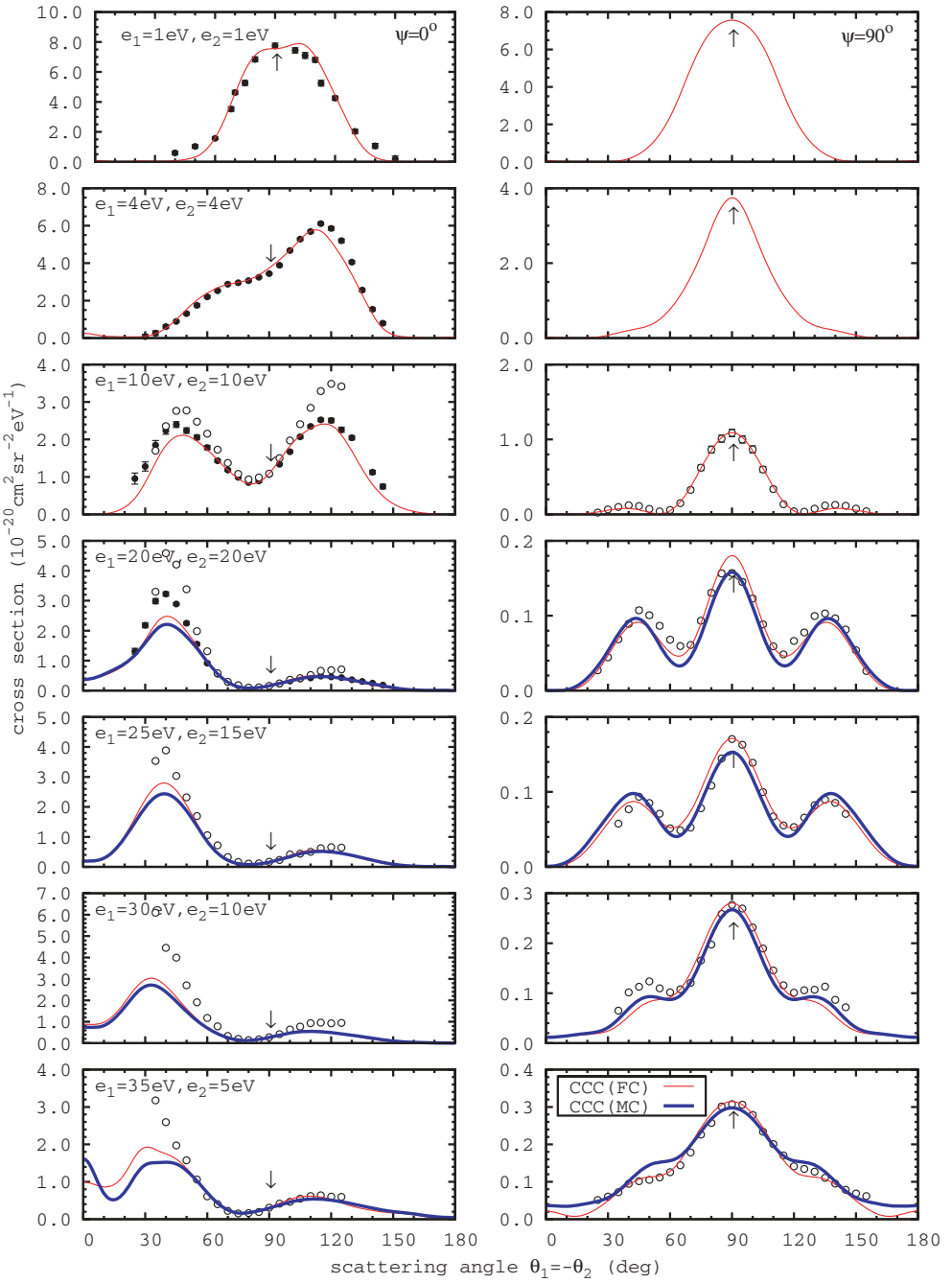

FIG. 2. (Color online) Fully differential cross sections for electron-impact single ionization of helium with outgoing electrons of the specified energies e_1 and e_2. The left panels are for the coplanar data, and the right panels are for the perpendicular-plane data. The arrows indicate the $\theta_1 = 90^\circ$ common point of both geometries; see Fig. 1. The experimental data shown by solid circles are from Refs. [26,27,29,32], and the data shown by open circles are from Refs. [28,31]. The present calculation was obtained using the CCC theory, utilizing the FC and MC calculations; see text.

There is excellent absolute agreement of CCC with the data of Rioual *et al.* [29]. The data of Murray *et al.* [28] have been normalized to the CCC theory at $\theta_1 = 90^\circ$, near the minimum for this geometry, which also coincides with the experiment of Rioual *et al.* [29]. In doing so, we see that the two experiments differ somewhat in shape, with CCC agreeing best with the data of Rioual *et al.* [29]. However, turning to the perpendicular-plane geometry, we find excellent agreement between CCC and the experimental results of Murray *et al.* [28]. This is surprising, particularly because now the $\theta_1 = 90^\circ$ point corresponds to the maximum for this geometry. In other words, we have the very unusual situation of having excellent agreement with a particular experiment for the smallest measured cross sections and poorest agreement for the largest.

This situation is also evident in the following four rows, where the outgoing electrons share the excess energy of 40 eV. The equal-energy-sharing case was studied in Stelbovics

et al. [19], and the asymmetric-energy-sharing cases were presented only recently [30]. Both studies utilized the FC treatment of He, where all appropriately symmetrized states have the He^+ 1*s* orbital describing one of the two electrons. Given the significance of the present discussion, we eliminate this approximation as a possible source of the identified discrepancies with experimental results. Accordingly, we present our first MC calculations for differential ionization. The ones presented have $n \leqslant 3$ short-ranged *s* and *p* orbitals in the configurations for the "inner" electron, which significantly improve the ground-state energy (0.1-eV error). Unfortunately, MC calculations often require an order of magnitude greater computational resources. This is due to the fact that we have to retain all states that arise from the multitude of configurations defined using the Laguerre-based orbitals [11]. We deliberately utilized the same orbitals in the corresponding FC and MC calculations so that the difference between the two was solely due to the different treatment of the core and the incident-energy variation. Consequently, the present FC calculations had to be chosen to be a little smaller than those reported by Bray *et al.* [30] so as to allow the corresponding MC calculations to be performed. The insignificant difference between the two calculations indicates that the FC approach to the problem suffices.

Beginning with the equal energy sharing ($e_1 = e_2 = 20\,\text{eV}$), we see a similar situation as for $e_1 = e_2 = 10\,\text{eV}$. The $\theta_1 = 90^\circ$ point is barely visible near the minimum of the coplanar geometry but is at the maximum of the perpendicular-plane geometry. Agreement with the experimental results of Murray and Read [31] is extraordinarily good (within 0.02 of the presented units) for the small cross sections in the latter geometry and yet differs from this experiment by two units at the maximum for the coplanar case. Agreement with the coplanar data taken by Röder [32] is much better.

The next three cases are for asymmetric energy sharing, and we find once more that agreement is best for the smallest perpendicular-plane cross sections rather than the largest coplanar ones. The last case considered, $e_1 = 35\,\text{eV}$ and $e_2 = 5\,\text{eV}$, is particularly interesting. Whereas for all of the cases presented the forward angles yielded very small cross sections, for this kinematical combination this region yields nearly the maximal cross section. This region is also rather sensitive to computational parameters and shows the largest variation in the two models.

IV. CONCLUSIONS

To summarize, there has been much progress in the field of electron-atom ionization in recent years. Most unusually, the progress first came from numerical treatments of the problem [2,3,7,19], without formal justification. Only following these computational methods has the few-body problem with Coulomb potentials been addressed to explain their success [16,17]. Even so, here we have identified some systematic discrepancies with experimental results, which are most unusual. Whereas it is common for theories to yield agreement with experimental results for the largest cross sections but not the smallest, we found the complete opposite situation, with the smallest cross sections obtained with great accuracy while having substantial discrepancy with the largest cross sections. The discrepancies cannot be resolved utilizing the MC treatment of the target.

Theories become truly valuable when they are predictive. There have been several cases previously where the CCC theory has disagreed with experimental results that subsequently were shown to be due to problems with the experiment. Examples include electron-hydrogen scattering [12,33–36] and double photoionization of helium [37,38]. We hope that this work will generate interest from experimentalists and other theorists to test the CCC results presented here. Should the CCC results be validated, then we have a very strong case for claiming that the *e*-He single-ionization (and excitation) problem has been solved.

ACKNOWLEDGMENTS

We thank A. J. Murray for providing his data in electronic form. This work was supported by the Australian Research Council. We are grateful for access to the Australian National Computing Infrastructure Facility and its Western Australian node iVEC.

[1] I. Bray and D. V. Fursa, Phys. Rev. Lett. **76**, 2674 (1996).
[2] T. N. Rescigno, M. Baertschy, W. A. Isaacs, and C. W. McCurdy, Science **286**, 2474 (1999).
[3] M. Baertschy, T. N. Rescigno, and C. W. McCurdy, Phys. Rev. A **64**, 022709 (2001).
[4] P. L. Bartlett, A. T. Stelbovics, and I. Bray, J. Phys. B **37**, L69 (2004).
[5] P. L. Bartlett, J. Phys. B **39**, R379 (2006).
[6] J. Colgan and M. S. Pindzola, Phys. Rev. A **74**, 012713 (2006).
[7] I. Bray, Phys. Rev. Lett. **89**, 273201 (2002).
[8] J. Colgan, M. Foster, M. S. Pindzola, I. Bray, A. T. Stelbovics, and D. V. Fursa, J. Phys. B **42**, 145002 (2009).
[9] T. F. O'Malley, P. G. Burke, and K. A. Berrington, J. Phys. B **12**, 953 (1979).
[10] K. Bartschat, E. T. Hudson, M. P. Scott, P. G. Burke, and V. M. Burke, J. Phys. B **29**, 2875 (1996).
[11] D. V. Fursa and I. Bray, Phys. Rev. A **52**, 1279 (1995).
[12] I. Bray and A. T. Stelbovics, Phys. Rev. A **46**, 6995 (1992).
[13] I. Bray and A. T. Stelbovics, Phys. Rev. Lett. **70**, 746 (1993).
[14] D. V. Fursa and I. Bray, J. Phys. B **30**, 757 (1997).
[15] A. Crowe and I. Bray, in *Physics of Atoms and Molecules: Selected Topics in Electron Physics*, edited by D. M. Campbell and H. Kleinpoppen (Plenum, 1995), pp. 45–56 .
[16] A. S. Kadyrov, I. Bray, A. M. Mukhamedzhanov, and A. T. Stelbovics, Phys. Rev. Lett. **101**, 230405 (2008).
[17] A. S. Kadyrov, I. Bray, A. M. Mukhamedzhanov, and A. T. Stelbovics, Ann. Phys. **324**, 1516 (2009).
[18] I. Bray and D. V. Fursa, Phys. Rev. A **54**, 2991 (1996).
[19] A. T. Stelbovics, I. Bray, D. V. Fursa, and K. Bartschat, Phys. Rev. A **71**, 052716 (2005).
[20] I. Bray, Phys. Rev. Lett. **78**, 4721 (1997).
[21] A. T. Stelbovics, Phys. Rev. Lett. **83**, 1570 (1999).

[22] M. Schulz, R. Moshammer, D. Fischer, H. Kollmus, D. H. Madison, S. Jones, and J. Ullrich, Nature **422**, 48 (2003).
[23] M. Durr, B. Najjari, M. Schulz, A. Dorn, R. Moshammer, A. B. Voitkiv, and J. Ullrich, Phys. Rev. A **75**, 062708 (2007).
[24] M. Dürr, C. Dimopoulou, A. Dorn, B. Najjari, I. Bray, D. V. Fursa, Z. Chen, D. H. Madison, K. Bartschat, and J. Ullrich, J. Phys. B **39**, 4097 (2006).
[25] M. Durr, C. Dimopoulou, B. Najjari, A. Dorn, K. Bartschat, I. Bray, D. V. Fursa, Z. Chen, D. H. Madison, and J. Ullrich, Phys. Rev. A **77**, 032717 (2008).
[26] T. Rösel, J. Röder, L. Frost, K. Jung, H. Ehrhardt, S. Jones, and D. H. Madison, Phys. Rev. A **46**, 2539 (1992).
[27] I. Bray, D. V. Fursa, J. Röder, and H. Ehrhardt, Phys. Rev. A **57**, R3161 (1998).
[28] A. J. Murray, F. H. Read, and N. J. Bowring, Journal de Physique **3**, 51 (1993).
[29] S. Rioual, J. Röder, B. Rouvellou, H. Ehrhardt, A. Pochat, I. Bray, and D. V. Fursa, J. Phys. B **31**, 3117 (1998).
[30] I. Bray, T. Lepage, D. V. Fursa, and A. T. Stelbovics, J. Phys. B **43**, 074028 (2010).
[31] A. J. Murray and F. H. Read, J. Phys. B **26**, L359 (1993).
[32] I. Bray, D. V. Fursa, J. Röder, and H. Ehrhardt, J. Phys. B **30**, L101 (1997).
[33] H. A. Yalim, D. Cvejanovic, and A. Crowe, Phys. Rev. Lett. **79**, 2951 (1997).
[34] R. W. O'Neill, P. J. M. van der Burgt, D. Dziczek, P. Bowe, S. Chwirot, and J. A. Slevin, Phys. Rev. Lett. **80**, 1630 (1998).
[35] J. F. Williams and A. G. Mikosza, J. Phys. B **39**, 4113 (2006).
[36] J. F. Williams and A. G. Mikosza, J. Phys. B **39**, 4339 (2006).
[37] A. S. Kheifets and I. Bray, Phys. Rev. Lett. **81**, 4588 (1998).
[38] M. Achler, V. Mergel, L. Spielberger, R. Dorner, Y. Azuma, and H. Schmidt-Böcking, J. Phys. B **34**, 965 (2001).