

Ab initio treatment of electron capture by B^{4+} ions from atomic hydrogen

F. Fraija, A. R. Allouche, and M. C. Bacchus-Montabonel

Laboratoire de Spectrométrie Ionique et Moléculaire, Université Lyon I, 43, Boulevard du 11 Novembre 1918, 69622 Villeurbanne Cedex, France

(Received 13 July 1993)

Ab initio potential-energy curves and radial and rotational coupling matrix elements have been calculated by means of configuration-interaction methods. A semiclassical treatment including electron translation factors has been performed in the $(0.1-1.5) \times 10^8$ cm/s velocity range and provides a good agreement with experiment.

PACS number(s): 34.20.Mq, 34.70.+e

I. INTRODUCTION

Electron capture of multiply charged ions in collisions with neutral atoms is an important process in tokamak-produced fusion plasmas. In particular, the study of reactions involving carbon or oxygen ions has been stimulated by the need of precise informations about impurity-ion behavior. Nevertheless, relatively little attention has been paid so far to boron ions which could, however, play a quite important role.

In a general investigation on collisions involving boron ions in controlled nuclear fusion reactions, we have developed recently a complete theoretical treatment of the $B^{3+}(1s^2)+He(1s^2)$ reaction [1]. The study is now extended to the $B^{4+}(1s)+H(1s)$ collision using an *ab initio* method for the determination of the potential-energy curves and couplings, well-adapted for this open-shell system, followed by a semiclassical collisional treatment including electron translation effects.

Few experimental data are available for this system. The measurements of Gardner *et al.* [2] and Crandall, Phaneuf, and Meyer [3] show, however, a quite efficient single electron-capture process in the intermediate energy range. From a theoretical point of view, the $B^{4+}(1s)+H(1s)$ system remains unexplored. In a complete theoretical investigation, we have thus considered the $^{1,3}\Sigma^+$ states correlated to the entry channel and the $\{B^{3+}(1s,3l)+H^+\}$ configuration, as well as the corresponding $^{1,3}\Pi$ and $^{1,3}\Delta$ states correlated to the $\{B^{3+}(1s,3l)+H^+\}$ exit channels.

II. COMPUTATIONAL METHOD

The potential-energy curves of the states of interest have been calculated in the interatomic distance range 1.5–20 a.u. by means of an *ab initio* method with configuration interaction using the CIPSI (configuration interaction by perturbation of a multiconfiguration wave function selected iteratively) algorithm [4]. Relatively compact configuration-interaction spaces have been used in the calculation (231 determinants for the $^{1,3}\Sigma^+$ states, 120 determinants for the $^{1,3}\Pi$ states, and 86 determinants for the $^{1,3}\Delta$ states) ensuring a fair description of the zeroth-order Hamiltonian with a threshold $\eta=0.005$ for

the perturbation contribution. The atomic basis set has been constructed from Gaussian functions. For boron we have used the $6s, 3p, 1d$ basis previously optimized for the $B^{3+}(1s^2)+He(1s^2)$ collisional system [1] added of one p and one d diffuse function with an exponent of 0.0095 and 0.2, respectively. For hydrogen we used the $4s, 2p$ basis determined from Huzinaga [5] by Chambaud *et al.* [6]. This basis provides a quite good agreement with experiment [7] for the B^{3+} energy levels (Table I), reproducing in particular the relative position of the $B^{3+}(1s3p)$ and $B^{3+}(1s3d)$ energy levels in both triplet and singlet multiplicities, the asymptotic separation energy is nevertheless less accurate for singlet than for triplet states. The discrepancy is, however, never more than 0.26 eV which represents a good accuracy compared with previous applications [8,9]. The most difficult levels to reproduce are the $B^{3+}(1s3p)$ levels which show a rather important gap between singlet and triplet multiplicities.

The radial coupling matrix elements $g_{KL}(R) = \langle \Psi_K | (\partial/\partial R) \Psi_L \rangle$ between all pairs of states of the same symmetry have been calculated by means of the finite-difference technique:

$$g_{KL}(R) = \lim_{\Delta \rightarrow 0} (1/\Delta) \langle \Psi_K(R) | \Psi_L(R + \Delta) \rangle,$$

with a parameter $\Delta=0.0012$ a.u.

The method has been extended to the calculation of the quadrupole moment tensor between electronic wave functions leading to a direct determination of the rotational

TABLE I. Comparison of the calculated atomic energy levels with the experimental values of Bashkin and Stoner [7] (in a.u.).

Atomic level	Energy	
	<i>Ab initio</i> calculation	Experiment
$B^{4+}(1s)$	9.5094	9.5391
$B^{3+}(1s3p)^1P$	8.6487	8.6553
$B^{3+}(1s3d)^1D$	8.6486	8.6499
$B^{3+}(1s3d)^3D$	8.6484	8.6499
$B^{3+}(1s3p)^3P$	8.6369	8.6271
$B^{3+}(1s3s)^1S$	8.5909	
$B^{3+}(1s3s)^3S$	8.5892	8.5838
$B^{3+}(1s^2)^1S$	0.0	0.0

coupling matrix elements and the consideration of translation effects in the collision dynamics. In the approximation of the common translation factor developed by Errea, Mendez, and Riera [10], the radial and rotational coupling matrix elements between states Ψ_K and Ψ_L may indeed be transformed, respectively, into [11]

$$\langle \Psi_K | \frac{\partial}{\partial R} - (\epsilon_K - \epsilon_L) z^2 / 2R | \Psi_L \rangle ,$$

$$\langle \Psi_K | iL_y + (\epsilon_K - \epsilon_L) z x | \Psi_L \rangle ,$$

where ϵ_K and ϵ_L are the electronic energies of states Ψ_K and Ψ_L , and z^2 and zx are the components of the quadrupole moment tensor. This expression is applicable for any choice of the origin of the electronic coordinates. We have taken the boron nucleus as origin of electronic coordinates in the molecular structure calculation.

III. MOLECULAR RESULTS

The potential-energy curves of the $^1,3\Sigma^+$ states are displayed, respectively, in Figs. 1(a) and 1(b). For both

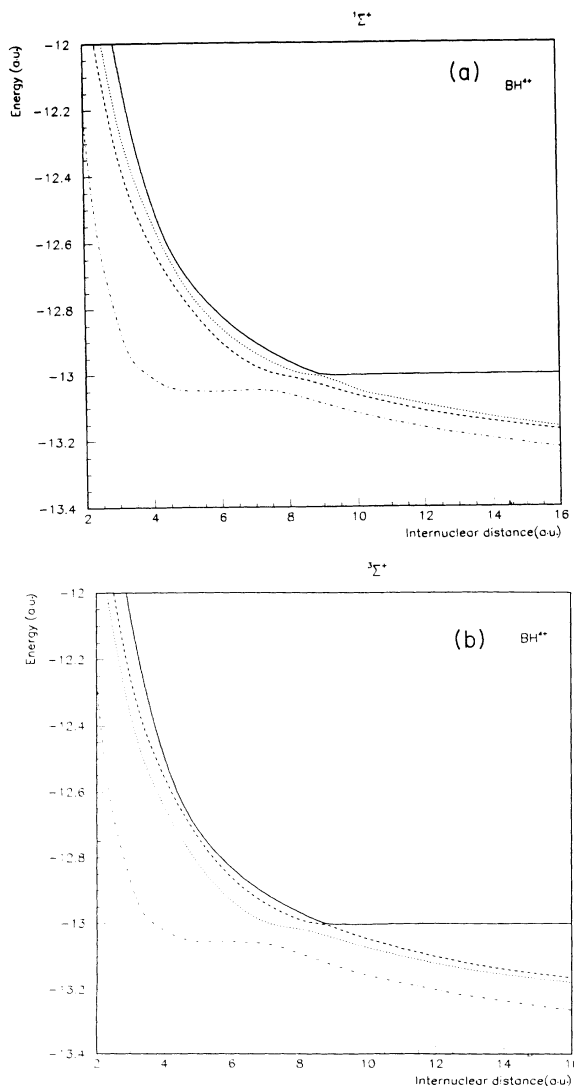


FIG. 1. Adiabatic potential-energy curves of the Σ^+ states of BH^{4+} . (a) Singlet states; (b) triplet states. —, $B^{4+}(1s)+H(1s)$; — —, $B^{3+}(1s3d)+H^+$; ····, $B^{3+}(1s3p)+H^+$; - · - ·, $B^{3+}(1s3s)+H^+$.

multiplicities, the potentials show a very sharp avoided crossing at a relatively long distance, but the states involved are not the same. The crossing appears between the entry channel and the $\{B^{3+}(1s,3p)+H^+\}$ channel for singlet states, when it occurs between the entry channel and the $\{B^{3+}(1s,3d)+H^+\}$ channel for triplet states. This is a direct consequence of the relative position of the atomic energy levels already mentioned in Table I. More precisely, this avoided crossing may be observed at $R=8.9$ a.u. with a separation energy at a crossing point of 5.7×10^{-3} a.u. for singlet states, and at $R=8.8$ a.u. with a separation energy of 3.710^{-3} a.u. for triplet states. These values of the separation energy at the crossing

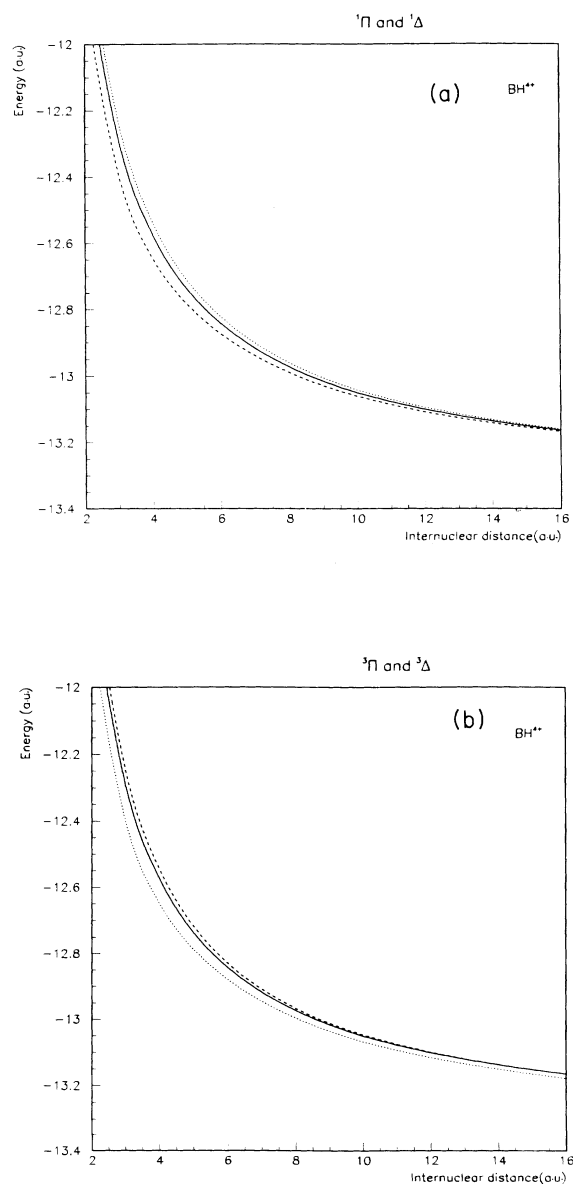


FIG. 2. Adiabatic potential-energy curves for the Π and Δ states of BH^{4+} . (a) Singlet states; (b) triplet states. —, $^1,3\Delta$ states correlated to $\{B^{3+}(1s3d)+H^+\}$; — —, $^1,3\Pi$ states correlated to $\{B^{3+}(1s3d)+H^+\}$; ····, $^1,3\Pi$ states correlated to $\{B^{3+}(1s3p)+H^+\}$.

point are of the same order as the precision of the calculation, about 10^{-3} a.u. and are thus obtained with a relatively large uncertainty. This problem has already been pointed out in the case of the $B^{3+}(1s^2)+He(1s^2)$ system [1] for which the assumption of a diabatic outer crossing has been shown to be quite correct. The potential-energy curves of the $1,3\Pi$ and $1,3\Delta$ states are displayed in Figs. 2(a) and 2(b) and show roughly the same features with no evidence of any avoided crossing.

The radial coupling matrix elements between $1,3\Sigma^+$ states are sketched in Figs. 3(a) and 3(b). They show sharp peaks for singlet and triplet multiplicities, respectively, 3.4 and 4.8 a.u. high, in correspondence with the

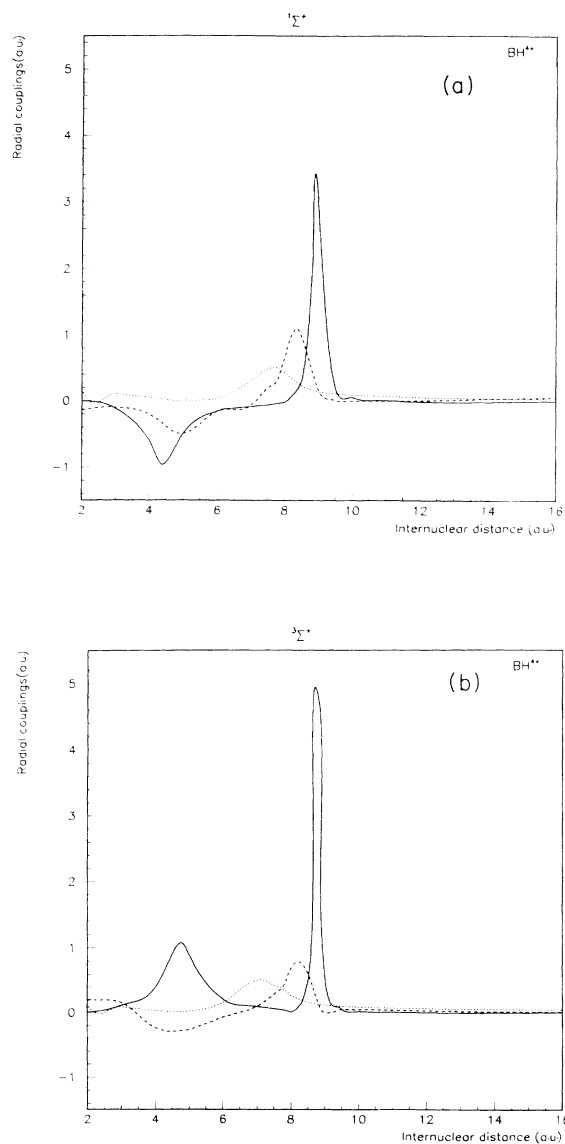


FIG. 3. Radial coupling matrix elements between Σ states. (a) Singlet states: —, $\langle 3p | \partial/\partial R | 1s \rangle$; ---, $\langle 3d | (\partial/\partial R) | 3p \rangle$; ···, $\langle 3s | (\partial/\partial R) | 3d \rangle$. (b) Triplet states: —, $\langle 3d | (\partial/\partial R) | 1s \rangle$; ---, $\langle 3p | (\partial/\partial R) | 3d \rangle$; ···, $\langle 3s | (\partial/\partial R) | 3p \rangle$.

avoided crossings at $R=8.9$ and 8.8 a.u. already observed on the potential-energy curves. A second peak about 1.0 a.u. high is observable on both multiplicities at shorter internuclear distances, respectively $R=4.4$ and 4.8 a.u. In the case of the $1\Sigma^+$ states, another significant peak is observable between the $B^{3+}(3p)$ and $B^{3+}(3d)$ channels; such a peak is markedly smaller for $3\Sigma^+$ states.

The rotational coupling matrix elements are displayed in Figs. 4(a) and 4(b) for singlet states and in Figs. 5(a) and 5(b) for triplet states. At large internuclear distances, rotational couplings are seen to be rather large for Π and Σ states corresponding to the same configuration; i.e., the $\{B^{3+}(1s, 3p)+H^+\}$ and $\{B^{3+}(1s, 3d)+H^+\}$ levels. In connection with the inversion of the $3p$ and $3d$ levels between the singlet and triplet multiplicities, a great similarity can be observed in Figs. 4(a) and 5(b) on the one hand, and in Figs. 4(b) and 5(a) on the other hand. The role of the $3d$ and $3p$ levels is interchanged when moving from the singlet to the triplet manifold.

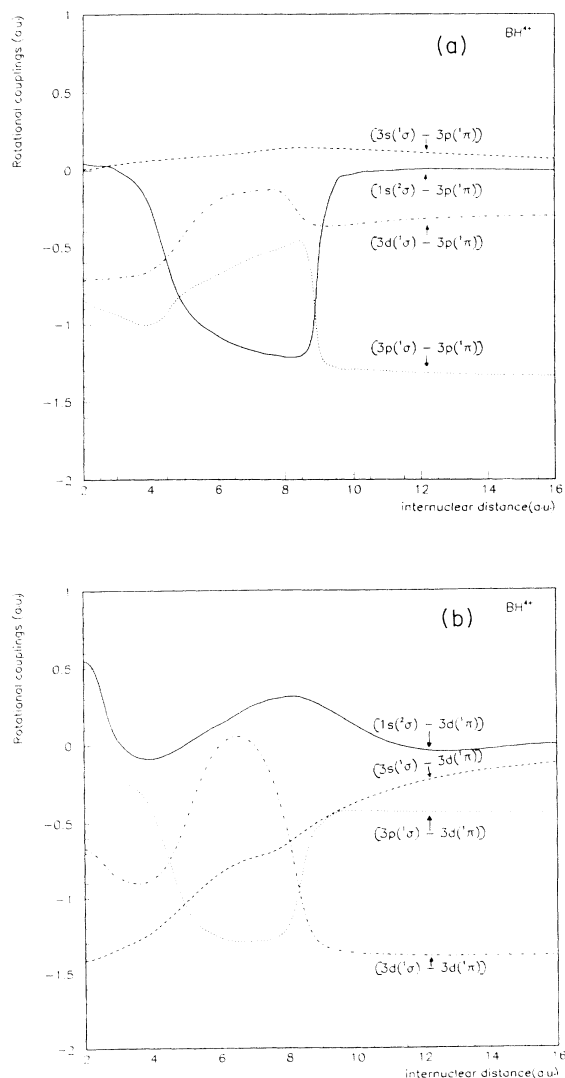


FIG. 4. (a), (b) Rotational coupling matrix elements between $1\Sigma^+$ and 1Π states.

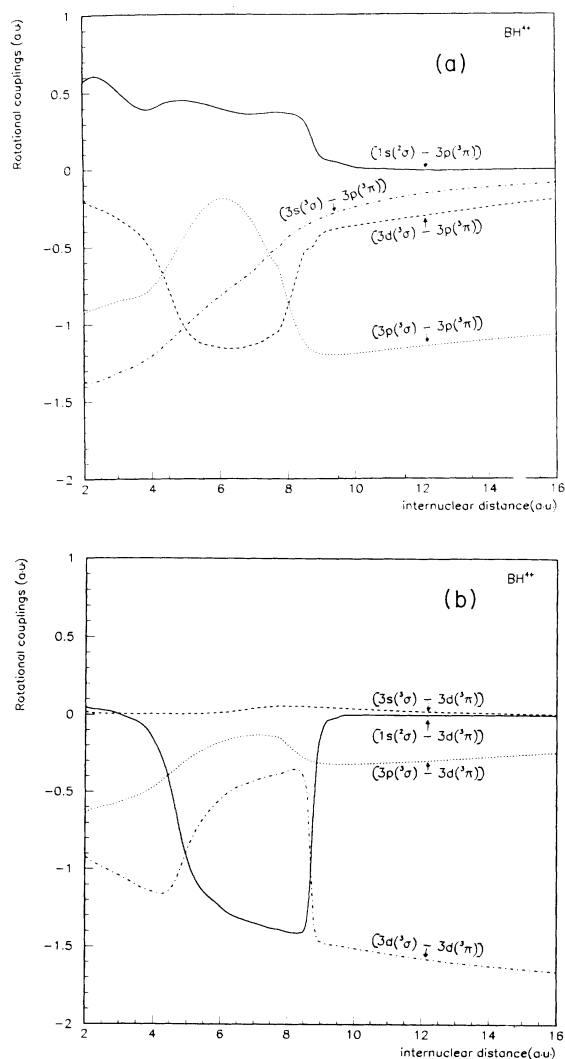


FIG. 5 (a),(b) Rotational coupling matrix elements between $^3\Sigma^+$ and $^3\Pi$ states.

IV. COLLISION DYNAMICS

The collision dynamics has been treated by semiclassical methods which should be valid down to about 10 eV amu^{-1} . The EIKONXS computer program [12] including the common translation factors of Errea, Mendez, and Riera [10] has been used. The coupled equations have been integrated separately for singlet and triplet states and the cross sections have been determined according to the statistical weights $\frac{1}{4}$ and $\frac{3}{4}$, respectively. The calculation has been performed in the $(0.1-1.5) \times 10^8 \text{ cm/s}$ velocity range in order to reach the collision energies used in experimental measurements. The total and partial capture cross sections including common translation factors and rotational couplings are presented in Fig. 6 and compared with the results obtained with only radi-

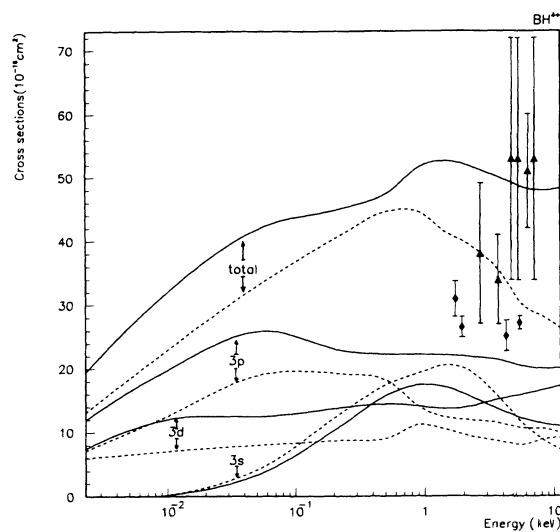


FIG. 6. Total and partial cross sections for the $B^{4+} + H$ system as a function of the center of mass energy. —, radial and rotational coupling; ---, radial coupling; ▲, Gardner *et al.* [2]; ◆, Crandall, Phaneuf, and Meyer [3].

al couplings. In fact no important translation effect appears for this system but a quite significant rotational effect is exhibited for the $3p$ and $3d$ channels. For the $3d$ level, it appears to be merely constant all over the collision energy range, but for the $3p$ level it increases from about $E_{c.m.} = 0.5 \text{ keV}$ leading to a noticeable effect over the total cross section. Our results are in quite good accordance with the experimental measurements of Gardner *et al.* [2] which overestimate by about 40% the results of Crandall, Phaneuf, and Meyer [3]. It seems clear that some uncertainties remain over the experimental data and some further measurements should be useful to complete the comparison.

V. CONCLUDING REMARKS

This work provides a complete determination of the potential-energy curves and radial and rotational coupling matrix elements for the $B^{4+}(1s) + H(1s)$ collisional system. In agreement with the experimental data, an inversion of the $3p$ and $3d$ atomic and molecular energy levels is observable for the singlet states. The total capture cross sections show a reasonable agreement with experiment at relatively high collisional energies. Some further measurements, in particular at lower energies, should be welcome to complete the discussion.

ACKNOWLEDGMENT

The Laboratoire de Spectrométrie Ionique et Moléculaire is "Unité Associée No. 171 au CNRS."

[1] F. Fraija, M. C. Bacchus-Montabonel, and M. Gargaud, *Z. Phys. D* (to be published).

[2] L. D. Gardner, J. E. Bayfield, P. M. Koch, I. A. Sellin, D. J. Pegg, R. S. Peterson, and D. H. Crandall, *Phys. Rev. A*

21, 1397 (1980).

[3] D. H. Crandall, R. A. Phaneuf, and F. W. Meyer, *Phys. Rev. A* **19**, 504 (1979).

[4] B. Huron, J. P. Malrieu, and P. Rancurel, *J. Chem. Phys.*

- 58, 5745 (1973).
- [5] S. Huzinga, *J. Chem. Phys.* **42**, 1293 (1965).
- [6] G. Chambaud, P. Millié, J. Ridard, and B. Lévy, *J. Phys. B* **12**, 221 (1979).
- [7] S. Bashkin and J. O. Stoner, *Atomic Energy Levels and Grotian Diagrams* (North-Holland, Amsterdam, 1975).
- [8] M. C. Bacchus-Montabonel, *Phys. Rev. A* **36**, 1994 (1987); **46**, 217 (1992); K. Amezian and M. C. Bacchus-Montabonel, *Chem. Phys. Lett.* **155**, 199 (1989); **199**, 487 (1992).
- [9] B. Zygelman, D. L. Cooper, M. J. Ford, A. Dalgarno, J. Gerratt, and M. Raimondi, *Phys. Rev. A* **46**, 3846 (1992).
- [10] L. F. Errea, L. Mendez, and A. Riera, *J. Phys. B* **15**, 101 (1982).
- [11] M. Gargaud, Doctorate thesis, University of Bordeaux-France, 1987 (unpublished).
- [12] R. J. Allan, Daresbury Laboratory Technical Memorandum No. G90/344, 1990 (unpublished); R. J. Allan, C. Courbin, P. Salas, and P. Wahnon, *J. Phys. B* **23**, L461 (1990).