Quasimolecular bremsstrahlung in heavy-ion collisions

R. Anholt*
Department of Physics, Stanford University, Stanford, California 94305

A. Salin†
Université de Bordeaux I, Laboratoire d'Astrophysique, 33405 Talence, France
(Received 14 January 1977)

In heavy-ion collisions, the molecular electronic dipole moment is accelerated and may emit continuum x rays even in the absence of inner-shell vacancies. Semiclassical calculations of the bremsstrahlung intensity are made for 200-MeV Kr + Ti encounters using hydrogenic two-center wave functions to calculate the molecular dipole moment. The bremsstrahlung is confined to x-ray energies below the Kr K x-ray lines.

One of the main problems in interpreting noncharacteristic continuum radiation observed in heavy-ion-atom encounters is to calculate the intensities from various bremsstrahlung processes,[1-3] as well as the intensity of molecular-orbital (MO) x rays.[4] Nucleus-nucleus bremsstrahlung, emitted by the accelerated dipole between the nuclear charges, has received much attention.[2,5] Recently, Chen *et al.*[6] suggested that a new kind of background radiation may be present called "collective radiation." The radiation is emitted because "during the collision, electrons can be induced to radiate because of the distortion of the charge densities and the coupling of the radiation field with the nuclear motion."[6] We interpret this radiation classically; the radiation is emitted because of the acceleration of the electronic dipole moment during the collision.

The molecular model of heavy-ion collisions[7] holds that the electronic wave functions during a collision will not be simple atomic orbitals of the projectile and target, but will combine to form diatomic molecular orbitals. Hence the electronic dipole moment will not be the difference between the number of projectile and target electrons (ΔN) multiplied by the internuclear distance (R), but in general will be less since part of the projectile's electron density will be shared with the target and vice versa. Because the molecular wave functions depend on internuclear distance, the molecular electronic dipole moment has not only a first time derivative, but also a second time derivative. The dipole moment is accelerated (even in the absence of Coulomb deflection, $\ddot{R}=0$); hence it can emit radiation.

In this communication, we perform semiclassical calculations of the x-ray intensity emitted in 200-MeV Kr + Ti encounters. Previously, Levine and Birnbaum[8] considered this type of bremsstrahlung in collisions between inert-gas atoms at thermal velocities where the radiation was observed in the infrared. Part of our analysis is similar to theirs. Chen *et al.*[6,9] presented a quantum-mechanical theory of this process. However, they did not make calculations of the x-ray intensity; hence the importance of this process could not be properly evaluated. We shall show that the molecular bremmstrahlung intensity is generally negligible compared to the intensity of x rays from the filling of molecular inner-shell vacancies ("MO x rays").

The total electric dipole moment of the quasimolecule calculated in the center-of-mass (CM) frame at time t is given by the sum of a nuclear and an electronic component:

$$\begin{aligned}\vec{\mu}_{\text{tot}}(t) &= \vec{\mu}_N(R(t)) + \vec{\mu}_e(R(t)) \\ &= (Z_1/A_1 - Z_2/A_2)A_r e\vec{R}(t) \\ &\quad + \sum_i \langle \psi_i(\vec{r},\vec{R}(t)) | e\vec{r} | \psi_i(\vec{r},\vec{R}(t)) \rangle, \end{aligned} \tag{1}$$

where Z_1 (Z_2) and A_1 (A_2) are the projectile (target) atomic and mass numbers, $A_r = A_1A_2/(A_1+A_2)$, and the sum i is over filled MO's $\psi_i(\vec{r},\vec{R}(t))$. The intensity of radiation emitted into all space per unit energy from the acceleration of this dipole is obtained by Fourier analyzing $\ddot{\mu}(t)$,[8,10]

$$I(\omega,b,v) = \frac{2\omega}{3\pi\hbar^2c^3}\left|\int_{-\infty}^{\infty}\dot{\vec{\mu}}(t)\,dt\,e^{i\omega t}\right|^2, \tag{2}$$

where $E_x = \hbar\omega$, b is the impact parameter, and v is the ion velocity. The differential cross section for x-ray emission is given by integrating I over impact parameters:

$$\frac{d\sigma}{dE_x} = \int_0^\infty 2\pi b\,db\,I(\omega,b,v). \tag{3}$$

The emission of photons requires $\ddot{\mu}(t)\neq 0$ at least for some values of t. The dipole component of the nucleus-nucleus bremsstrahlung (NNB) cross section has been obtained by Fourier analyzing the nuclear component of $\mu(t)$ along a Coulomb trajectory where $\ddot{R}(t)\neq 0$.[5]

This comment considers the electronic contribution to $\mu(t)$. For neutral-neutral encounters at large distances, this contribution must approach the same magnitude as the first term but with the opposite sign so that the expected result $\mu_{tot}(R \approx \infty) = 0$ is obtained. At $R = 0$ (or $R \ll a_K$, the K radius of the higher-Z collision partner), the electronic part must approach zero since the united atom has no dipole moment. If the electron clouds could be described by atomic orbitals throughout the entire collision, the dipole moment of the ith electron calculated from a point halfway between the two nuclei (center of the molecule) will be $\pm\frac{1}{2}eR(t)$, where the sign would depend upon which collision partner the electron was attached to. For intermediate distances, however, the electron clouds are distorted into MO's where part of the density is shifted toward the opposite collision partner. Hence, usually $|\mu_{ie}(R)|$ is less than $\frac{1}{2}eR$.

To calculate molecular dipole moments, it is necessary to shift from the CM to the center of the molecule (CMO). For diatomic molecules the electric dipole moment has only a z component (parallel to $\vec{R}$). Defining the shift $R_{\mathrm{CMO}} - R_{\mathrm{CM}} = \Delta$ we have, assuming ψ_i is orthonormal:

$$\vec{\mu}_{ie} = \hat{k}\langle\psi_i|z_{\mathrm{CM}}|\psi_i\rangle = \hat{k}\langle\psi_i|z_{\mathrm{CMO}}|\psi_i\rangle + \Delta\hat{k}. \tag{4}$$

Figure 1 shows electric dipole moments as a function of internuclear distance for various values of $Q = Z_1/Z_2$ or Z_2/Z_1, calculated using nonrelativistic one-electron two-center wave functions.[11] To display the variation of μ_{ie} with internuclear distance, we have subtracted $\mu_{ie} = \langle\psi_i|z_{\mathrm{CMO}}|\psi_i\rangle$ from $\frac{1}{2}eR$ as follows:

$$\mu'_{ie} = \mathrm{sgn}(\mu_{ie})[\tfrac{1}{2}eR - |\mu_{ie}|]. \tag{5}$$

The quantity μ'_{ie} conveniently approaches zero at both the separated-atom and united-atom limits. Figure 1 shows that the most weakly bound electron clouds are the most polarized (μ'_{ie} is largest). Also, the clouds are polarized more in near-symmetric ($Q = 1$) than in asymmetric encounters. For $Q = 1$, however, $\mu_{ie} = 0$; hence $\mu'_{ie} \to \infty$ as $R \to \infty$. [However, in that case $\mu_{tot}(\infty) = \mu_{tot}(t) = 0$ for all t, neglecting isotope effects.] Finally, we note that the $1s\sigma$ and $2p\sigma$ molecular dipole moments change most rapidly with internuclear distance.

The radiation from the acceleration of these electronic dipole moments is coherent with NNB [see Eqs. (1) and (2)]. However, we calculated the radiation intensity by Fourier analyzing $\mu_e(t)$ and squaring $\mu_e(\omega)$ separately (see comments below). Also, since the radiation is produced in collisions with impact parameters as large as a_K, which is much greater than the internuclear distance of closest approach in a head-on collision, we can use straight-line trajectories. Hence the quantity μ'_{ie} shown in Fig. 1 can be Fourier analyzed directly, neglecting $\frac{1}{2}eR$ in Eq. (5) and Δ in Eq. (4).

Figure 2 shows a numerical evaluation of the cross section for radiation emission in 200-MeV Kr + Ti encounters.[12] Clearly, the radiation is confined to low x-ray energies which are not measured in studies of K MO x rays (transitions to vacancies in the $1s\sigma$ MO, where E_x is greater than the binding energy of the heavier collision partner U_K). The contributions from the various dipole moments, Fourier analyzed and squared separately, are also shown. The total coherent sum of these contributions tends to be less than the incoherent sum, since the individual dipoles alter in sign, ex-

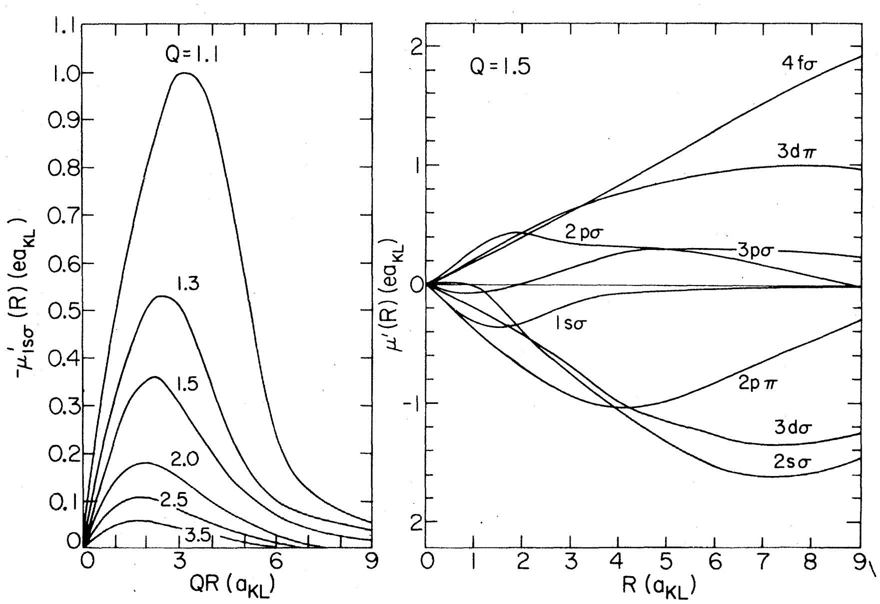

FIG. 1. (a) Electronic dipole moments for the $1s\sigma$ MO vs QR, where $Q(>1) = Z_1/Z_2$ or Z_2/Z_1. (b) Electronic dipoles for eight MO's and $Q = 1.5$ vs R in units of the lower-Z K radius. The $4f\sigma$, $3d\sigma$, and $3d\pi$ dipole moments have been divided by 2.

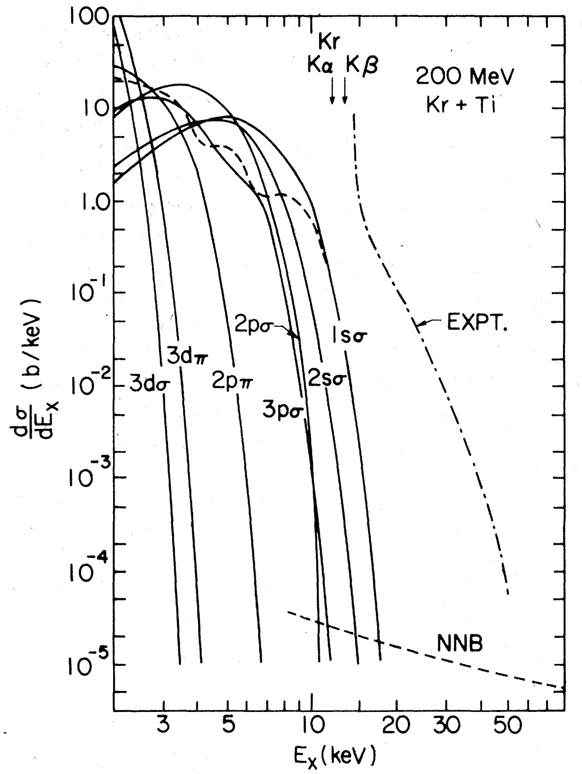

FIG. 2. Absolute cross sections for radiation emission in 200-MeV Kr+Ti collisions. The solid lines are calculations of the molecular bremsstrahlung from each MO considered separately. The dashed line is the coherent sum of the bremsstrahlung intensity from the lowest seven MO's. The NNB cross section and the experimentally observed continuum band are also shown.

cept for highly asymmetric encounters.

Only the innermost MO's are responsible for the highest energy radiation. This can be understood quantitatively if we parametrize $\mu'_{ie}(R)$ by $A\gamma eR \exp(-\gamma^2R^2)$.[8] This is reasonably valid for the $1s\sigma$ dipole (Fig.1), but less so for other dipole moments [one can also use a sum of terms $\sum_k A_k\gamma_k eR \exp(-\gamma_k^2R^2)$]. Using this parametrization, Eqs. (2) and (3) can be evaluated analytically so that the differential radiation cross section is given by

$$\frac{d\sigma}{dE_x}=\frac{2\pi\alpha}{3}\frac{A^2\beta^2}{E_x}q^2(q+1)e^{-q}, \tag{6}$$

where $\alpha=e^2/\hbar c$, $\beta=v/c$, and $q=\omega^2/(2\gamma^2v^2)$. The critical behavior of the cross section is contained in the factor e^{-q}. A large cross section is obtained either for low x-ray energies $\hbar\omega$, high velocities v, or large values of γ. The molecular dipole moment of the inner-shell electrons has the largest value of γ. To obtain a large cross section for $E_x > U_k$ and $v_1/v_k \ll 1$ (the ratio of the ion velocity to the K-electron velocity of the higher-Z collision partner), we require

$$q\approx\frac{1}{8}\left(\frac{E_x}{U_K}\right)^2\left(\frac{v_K}{v_1}\right)^2\frac{1}{(\gamma a_K)^2}\approx 1$$

or that $\gamma \gg a_K^{-1}$. It appears from Fig. 1 that this is rarely the case.

We should also note that the magnitude and x-ray energy dependence of NNB and of the quasimolecular bremsstrahlung are very different. Except near the crossover of the two curves in Fig. 2, it is clearly valid to consider the two processes separately, neglecting interference terms.

The example 200-MeV Kr+Ti was chosen because it has a large radiation cross section. In most examples which we have examined, the molecular bremsstrahlung is even less important. One possible exception is in 60-MeV I bombardments of Au, where low-energy ($6.5 < E_x < 9$ keV) "molecular M radiation" has been observed.[13] The integrated molecular bremsstrahlung cross section is 0.07 b compared to 10^3 b observed experimentally. Hence the 6.5–9-keV radiation observed in I+Au encounters is not molecular bremsstrahlung.

The electron bremsstrahlung considered in this paper is of quasimolecular origin, but unlike MO x rays, no vacancy need be present. We have shown that the electron dipole moment is not accelerated fast enough ($\gamma_{\max}\approx a_K^{-1}$) in collisions with $v_1/v_K \ll 1$ to allow the emission of high-energy photons. The bremsstrahlung is negligible compared with the intensity of x rays from transitions to inner-shell molecular vacancies. We doubt that this radiation can be observed at all, since the continuous radiation below the $K\alpha$ transitions in the heavier collision partner tends to be obscured by other kinds of bremsstrahlung, by MO L and M x rays, as well as by Compton-scattered separated-atom K x rays.

The authors wish to thank W. E. Meyerhof and J. C. Y. Chen for useful discussions. A. Salin acknowledges the hospitality of Stanford University and the Stanford Research Institute.

*Supported by the National Science Foundation.
†Equipe de recherche CNRS No. 137.

[1]R. Anholt and W. E. Meyerhof, in *Abstracts of the Fifth International Conference on Atomic Physics, Berkeley, 1976,* edited by R. Marrus, M. H. Prior, and H. A. Shugart (University of California, Berkeley, 1976), p. 60.
[2]H. P. Trautvetter, J. S. Greenberg, and P. Vincent,

Phys. Rev. Lett. 37, 202 (1976).
[3]R. Anholt and T. K. Saylor, Phys. Lett. 56A, 455 (1976).
[4]W. E. Meyerhof, T. K. Saylor, S. M. Lazarus, A. Little, B. B. Triplett, L. F. Chase, Jr., and R. Anholt, Phys. Rev. Lett. 32, 1279 (1974).
[5]J. Reinhardt, G. Soff, and W. Greiner, Z. Phys. A 276, 285 (1976).
[6]J. C. Y. Chen, T. Isihara, and K. M. Watson, Phys. Rev. Lett. 35, 1574 (1975).
[7]M. Barat and W. Lichten, Phys. Rev. A 6, 211 (1972).
[8]H. B. Levine and G. Birnbaum, Phys. Rev. 154, 86 (1966).
[9]Our interpretation of the theory of Chen *et al.* (Ref. 6) was suggested, in part, by B. Müller (private communication).
[10]J. D. Jackson, *Classical Electrodynamics* (Interscience, New York, 1962), Chap. 14.
[11]K. Helfrich and H. Hartmann, Theor. Chim. Acta. (Berlin) 16, 263 (1970). We thank K. Helfrich for providing a copy of his computer code.
[12]R. Anholt and W. E. Meyerhof (unpublished).
[13]P. H. Mokler, H. J. Stein, and P. Armbruster, Phys. Rev. Lett. 29, 827 (1972); and Gesellschaft für Schwerionenforschung, Report No. GSI 73-11, 1973 (unpublished).