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CRITICAL REMARKS ON A SCALING LAW FOR INNER-SHELL
IONIZATION

B. MÜLLER, J. REINHARDT, W. GREINER, G. SOFF

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Gesellschaft für Schwerionenforschung mbH
Planckstr. 1 · Postfach 1105 41 · D-6100 Darmstadt 11 · Germany

Critical remarks on a scaling law for inner-shell ionization*

Berndt Müller, Joachim Reinhardt and Walter Greiner
Institut für Theoretische Physik, Johann Wolfgang Goethe-Universität,
D-6000 Frankfurt am Main, Robert-Mayer-Str. 10

and
Gerhard Soff
Gesellschaft für Schwerionenforschung, Postfach 100 541
D-6100 Darmstadt

Abstract:

In superheavy quasimolecules the number of created $1s$ -vacancies per collisions P_{1s} can be evaluated approximately by a simple scaling law. This analytical relation correctly reproduces the measured dependence of P_{1s} on the impact parameter, bombarding energy and combined nuclear charge $Z=Z_1+Z_2$. It is emphasized, however, that the absolute ionization magnitude is underestimated typically by a factor of four. This discrepancy has been successfully resolved by the inclusion of multi-step excitation processes. It is shown that the theoretical derivation of the normalization constant in a previously reported scaling law is incorrect.

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1. Introduction

Collisions of very heavy ions with bombarding energies close to the Coulomb barrier offer us the possibility to perform a spectroscopy of electronic states in transient superheavy systems within the charge range of $108 \leq Z \leq 190$ ($g_2U + g_8Cf$). The pivotal question to answer is whether the binding energy of the strongest bound electronic state can reach or exceed twice the electron rest mass. An important task in this connection is the investigation of electron excitation processes in superheavy systems. Furthermore, ionization of the lowest quasimolecular boundstates represents an essential prerequisite for the occurrence of many atomic phenomena in heavy-ion collisions, such as positron creation, characteristic K-X-rays, delta electrons and quasimolecular K-X-rays. Various calculations have shown that the probability for the creation of a vacancy in such a collision is an extremely sensitive function of impact parameter b , relative impact velocity v , as well as of the magnitude of the binding energy and localization of the wave-function during the collision. It is, therefore, an obvious aim to derive a simple, analytical relationship among these quantities that replaces the original scaling law of Bang and Hansteen¹⁾ and its extensions²⁻³⁾, which is valid only for very asymmetric, light collision systems. The first scaling law being directly applicable to lso-ionization in superheavy quasimolecules was derived by several of us⁴⁾ within the framework of first-order time-dependent perturbation theory. It reproduced the dependence of the ionization probability on kinematical variables but did not yield the correct absolute magnitude.

In this paper we shall present a more elaborated version of this scaling law which basically confirms our former results. The authors of refs. 5) and 6) claimed that they obtained a theoretical expression for $P_{lso}(b)$ which

generally agrees with the experimental data except for the very heavy Pb+Cm colliding system. We will show that the normalization of this relation is not justified theoretically and thus should be considered as a fit constant.

2. Physical ingredients

We start our considerations from time-dependent perturbation theory within the quasimolecular basis. Here the transition amplitude from the initial $1s\sigma$ -state with the energy eigenvalue $E_{1s\sigma}$ to a final continuum state with an energy E is simply determined by ⁴⁾

$$a(E) = - \int_{-\infty}^{\infty} dt \langle \psi_E | \frac{\partial}{\partial t} | \psi_{1s\sigma} \rangle \exp \left\{ \frac{i}{\hbar} \int_{-\infty}^t dt' (E - E_{1s\sigma}') \right\} \quad (2.1)$$

The presence of additional electrons as well as the possible occurrence of multi-step excitation processes are already neglected in that treatment. Furthermore we remark that perturbation theory violates unitarity and eq. (2.1) thus should be applied only to collisions with rather small excitation probabilities. In the following derivation we make use of some characteristic features valid for all superheavy quasimolecules:

(a) Ionization takes place predominantly at very small internuclear distances, where the monopole approximation provides a good approximation to the binding energies of, and transition matrix elements between, quasimolecular states.

(b) Ionization of the $1s\sigma$ -level is dominated by radial coupling. The rotational coupling does not seem to play an important role because the relevant matrix elements vanish at small distances. In consequence we replace $\partial/\partial t$ by $\dot{R} \partial/\partial R$, where $\dot{R}$ denotes the radial ion velocity.

(c) The radial coupling matrix elements $\langle f | \partial/\partial R | i \rangle$ exhibit a strong peak at the point of closest approach of the two nuclei. The detailed shape of these matrix elements at large internuclear separations, especially the choice of translation factors seems to be only of minor importance.

Assuming point-like nuclei, a reasonable parametrization of the radial matrix elements is achieved by

$$\langle E\sigma' | \partial/\partial R | 1s\sigma \rangle = \frac{d(E,Z)}{R} \quad (2.2)$$

which is valid for small and intermediate distances R . E is the total energy of the emitted electron and $Z = Z_1 + Z_2$ is the combined nuclear charge of the system.

(d) The matrix element is a smooth function of E . The electrons are mainly ionized into states with less than 1 MeV kinetic energy. The transition strength in this range can be approximated by

$$d(E,Z) = d_0(Z) \left(\frac{m c^2}{E} \right)^{\gamma/2} \quad (2.3)$$

where γ is a slowly varying function of Z . The quantities d and γ are given in ref. 4). They may be evaluated employing the parametrization

$$\gamma(Z) = 2.08 - 0.024 (Z-140) \quad (2.4)$$

$$D(Z) = 1.2 + 0.054 (Z-158) - 0.000015 (Z-158)^3 \quad (2.5)$$

and

$$D(Z) = 4\pi^2 d_0^2 m c^2 \quad (2.6)$$

The amplitude for ejecting an electron from the $1s\sigma$ state into the continuum then takes the form

$$a(E) = - d \int_{-\infty}^{\infty} dt \frac{\dot{R}(t)}{R(t)} \exp \left\{ \frac{i}{\hbar} \int_{-\infty}^t dt' [E - E_{1s\sigma'}(R(t'))] \right\} \quad (2.7)$$

If we change the integration variable it may easily be transformed into

$$a(E) = - 2i d \int_{R_0}^{\infty} dR \frac{1}{R} \sin \left\{ \frac{1}{\hbar} \int_{R_0}^R dR' \frac{(E - E_{1s\sigma'}(R'))}{\dot{R}(R')} \right\}. \quad (2.8)$$

For a Coulomb trajectory the radial velocity is given by

$$\dot{R}(R) = \frac{v}{R} \sqrt{(R-R_0)(R+R_0 - 2a)} \operatorname{sgn}(t) \quad (2.9)$$

with the distance of closest approach

$$R_0 = a + \sqrt{a^2 + b^2}, \quad a = \frac{Z_1 Z_2 e^2}{2E_{CM}} \quad (2.10)$$

for impact parameter b , centre-of-mass bombarding energy E_{CM} and velocity v at infinity.

All excitations to high lying vacant bound states are neglected. In consequence the number of created $1s\sigma$ -vacancies per collision is determined by

$$P_{1s\sigma}(b) = 2 \int_0^\infty \frac{|a(E)|^2}{mc^2} dE \quad (2.11)$$

Using eq. (2.8) this can be written as

$$P_{1s\sigma}(b) = 8 d_0 \int_0^\infty \int_0^{\frac{mc^2}{E}} \gamma(Z) \left| \frac{1}{\pi} \int_{R_0}^\infty \frac{1}{R} \sin \left\{ \int_{R_0}^R dR' \frac{(E - E_{1s\sigma}(R'))}{\dot{R}(R')} \right\} \right|^2 dE \quad (2.12)$$

So far we followed our former treatment⁴⁾ of the scaling law and its modified representation of Bosch et al.⁶⁾

3. Derivation of the scaling law

A crude estimate of the integral (2.7) can be obtained from an investigation of the singularities of the integral $\dot{R}(t)/R(t)$ in the complex time plane. First, let us, for convenience, replace the variable transition energy in the phase of eq. (2.7) by its value at the distance of closest approach:

$$\Delta E_0 = E - E_{1s\sigma}(R_0).$$

From the equation of motion

$$\ddot{R} = v^2 \left[\frac{a}{R^2} - \frac{b^2}{R^3} \right] \quad (3.1)$$

it is easy to show that $|R(t)|$ can at most grow as a quadratic polynomial in the limit $|t| \rightarrow \infty$. Therefore the integration contour in Eq. (2.7) can be closed in the upper half complex t -plane, reducing the integral to one around all singularities of the function $(\dot{R}/R)$ in this region (see Fig. 1).

From eqs. (2.9) and (3.1) one can prove that the only singular points of this function are the points where $R(t)$ vanishes. By integrating (2.9) into the inverse function $t(R)$, or by inspecting the parametric representation

$$R = a(\cosh(\xi)+1), \quad t = \frac{a}{v} (\varepsilon \sinh(\xi) + \xi) \quad (3.2)$$

(with the eccentricity $\varepsilon = (R_0 - a)/a$), it is found that all zeroes of $R(t)$ must lie on the imaginary time-axis: the one closest to the origin being given by

$$\tau_0 = \text{Im}(t_0) = \frac{1}{v} \left[b - a \cos^{-1} \left(\frac{a}{R_0 - a} \right) + \pi a \right] =$$

$$\frac{1}{v} \left[b + a \left(\pi - \tan^{-1} \frac{b}{a} \right) \right]. \quad (3.3)$$

The quantity τ_0 can be regarded as the characteristic collision time of a

Coulomb trajectory. Similar expressions have been suggested by Backe and Kankeleit^{7,8}. The characteristic time $\tilde{t}$ defined by these authors differs from our τ_0 by less than 5% over the whole range of impact parameters.

The remaining integral is basically a small number, the dominant contribution coming from a pole term at $x=0$ that yields a factor π . The factor is slightly ϵ -dependent. One can therefore write approximately.

$$|a(E)|^2 \approx \pi^2 d_0^2 (mc^2/E)^\gamma \exp \left| -\frac{2\tau_0(E-E_{1so}(R_0))}{\hbar} \right| \quad (3.4)$$

Equation (3.4) reproduces the numerically known fact that the energy spectrum of ionized electrons falls off exponentially, apart from the weak energy dependence of the matrix element.

Following the approach of Bosch et al.⁽⁶⁾ one may get the same result with the exception that τ_0 should be replaced by R_0/v . The integration over final continuum states leads to

$$P_{1so}(b) = \frac{1}{2} D(Z) N \exp \left\{ \frac{2\tau_0}{\hbar} E_{1so}(R_0) \right\} \quad (3.5)$$

with

$$N = \left(\frac{2\tau_0}{\hbar} \frac{mc^2}{mc^2} \right)^{\gamma-1} \Gamma(1-\gamma, \frac{2\tau_0}{\hbar} \frac{mc^2}{mc^2}) \quad (3.6)$$

Here $\Gamma(a,x)$ denotes the incomplete gamma function⁹⁾, which we computed according to

$$\Gamma(a,x) = \Gamma(a) - \gamma(a,x) \quad (3.7)$$

and

$$\gamma(a,x) = \frac{x^a}{a} e^{-x} {}_1F_1(1,1+a;x) \quad (3.8)$$

The confluent hypergeometric function ${}_1F_1(a,b;x)$ is easily determined by its series representation. The final result of the calculation of Bosch et al.⁽⁶⁾ would be eq. (3.5) with the substitution $\tau_0 \rightarrow R_0/v$. However, the authors of ref. 5) and 6) published the scaling law (3.5) with the modified integral value $\tilde{N}$

$$\tilde{N} = \exp \left\{ -\frac{2}{\hbar v} \frac{R_0}{mc^2} \right\} \quad (3.9)$$

This wrong normalization constant may be obtained, if one arbitrarily replaces the variable E in eq. (3.4) by the constant mc^2 and furthermore performs the approximation

$$\int_0^\infty \left(\frac{mc^2}{E} \right)^\gamma dE = \frac{mc^2}{\gamma(Z)-1} \sim mc^2 \quad (3.10)$$

Still, the authors claimed good agreement of their scaling law with the experimental data that exceed the exact results of first-order perturbation theory by a factor 3 to 5. The agreement was, however, accidentally caused by the incorrect normalization constant (3.9). In the derivation of the expression (3.5) we assumed that the transition energy $E - E_{1so}$ does not change with the time, which is, of course, also incorrect. This approximation, however, can be avoided, but the final results become fairly complicated and are not particularly illuminating. For further discussions we refer to the appendix of ref. 10.

4. Comparison of various models

The diverse versions of the scaling law for $1s\sigma$ ionization in superheavy quasimolecules are compared in fig. 2a and 3a. As example we consider the collision system $^{54}\text{Xe} + ^{82}\text{Pb}$ at $E_{\text{lab}} = 4.7 \text{ MeV/u}$ (fig. 2) and the very heavy system $^{82}\text{Pb} + ^{96}\text{Cm}$ at 5.9 MeV/u (fig. 3). The solid lines are the graphical representation of eq. (3.5) and (3.6). To be consistent with the parametrization of the radial matrix elements we used binding energies¹¹⁾ of the $1s\sigma$ -electron, which are evaluated for point nucleus potentials. In the computations of refs. 5) and 6) binding energies for screened potentials were employed. The dashed lines displays results which are obtained from eq. (3.5) with the substitution $\tau_0 \rightarrow R_0/v$. The present calculations may be compared with our old model, i.e. eq. (11) of ref. 4) (dotted lines). These three scaling laws exhibit almost the same exponential decline and coincide approximately in the absolute magnitude with the numerical integration of eq. (2.1) and (2.11)⁴⁾. The outcome of the latter calculations is displayed in fig. 2b and 3b (dashed lines). Here, it should be emphasized that no parametrization of the matrix elements or binding energies has been applied. In contrast to this Bosch's law (dashed-dotted lines) obviously exceeds our results by a substantial factor. This is simply caused by the different values (3.6) and (3.9), respectively, for the integration over final continuum states. We may conclude that Bosch's scaling law⁶⁾ strongly overestimates the correct theoretical result within first-order perturbation theory and cannot be derived rigorously in that framework. However, it reproduces the experimental data fairly well and thus needs a theoretical explanation. The gravest concern, whether any of the presented scaling laws are applicable towards a spectroscopic analysis of binding energies in superheavy quasimolecules, comes from the numerically established fact that ionization in these systems can only be understood through coupled-channel calculations^{12,13)}.

The fair agreement of the calculated $P_{1s\sigma}(b)$ in the considered collision systems (solid lines in fig. 2b and 3b) with the measured data^{5,14)} is demonstrated in ref. 13) and 15). More work must be invested to extract from these coupled calculations a scaling law which is justified theoretically.

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Figure Captions:

Fig. 1: Integration contour for eq. (2.7) in the complex time plane. All singularities are located on the imaginary axis.

Fig. 2: a) The number of created $1s\sigma$ -vacancies $P_{1s\sigma}(b)$ per collision as a function of the classical impact parameter b . The superheavy system $^{54}\text{Xe} + ^{82}\text{Pb}$ at $E_{\text{lab}} = 4.7$ MeV/u is considered. Comparison of various model calculations. The solid line displays the result of eq. (3.5). The dashed line shows the same with the replacement $\tau_0 \rightarrow R_0/v$. The dotted line indicates the model of ref. 4. The outcome of Bosch's law (eq. 3.5 with 3.9) is depicted by the dashed-dotted line.

b) The dashed line shows $P_{1s\sigma}(b)$ as the result of first order time-dependent perturbation theory, i.e. the direct numerical evaluation of eqs. (2.1) and (2.11). The outcome of our coupled channel calculations is given by the solid line.

Fig. 3: The same as in fig. 2 for the heavier system $^{82}\text{Pb} + ^{96}\text{Cm}$ at 5.9 MeV/u.

Fig. 2

Fig. 1

Fig. 3