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Shaking process due to nuclear recoil during heavy ion-atom collisions

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ABSTRACT

A theoretical study on the shaking process accompanying swift heavy ion-atom collisions is presented. Using the nonrelativistic hydrogenic wavefunctions, analytical expressions for the survival and shakeup/shakedown probability have been derived for the $K-$, $L-$ and $M-$shell electrons of hydrogen-like atomic systems. The resulting expressions are used to calculate the shaking and shakeup/shakedown probability in the typical case of the recoiling nucleus of the multielectron ($^{63}Cu^{+}$) and hydrogen-like ($^{63}Cu^{28+}$) atomic systems, respectively. Interestingly, it is found that the requirement of the high colliding energy for the suddenness of the perturbation, can well fulfill the limiting condition of the necessary nuclear recoil for finite electron shaking during the ion-atom collisions. Further, the dependence of the shaking probability on atomic number has been depicted, and it has emerged that for a particular value of the recoil energy per nucleon, the shaking processes are more significant in the lower atomic number region.

1. Introduction

In the recent decades, progressive work in terms of theoretical advancements and experimental developments has been done to understand the various charge changing processes during the collisions of partially stripped ions and neutral atoms. In this connection, interestingly, one can find a definitive role of quantum mechanical treatment during the ion-atom interactions when the corresponding atomic system goes through various direct and indirect interaction processes. These interactions successively or abruptly change the central nuclear potential and/or the electronic environment, which consequently results in the change of the charge states of the concerned atomic system. In a typical case, if the perturbation or net change in the system occurs abruptly enough, then the orbiting electrons may not respond so rapidly to reorganize themselves, which causes the electrons getting excited to the unoccupied bound states (shakeup/shakedown process) or the continuum states (shakeoff process). These processes are called shaking processes [1] and treated under the sudden approximation limit [2]. It is worth to note that a perturbation is called sudden if the time period (τ) of the perturbation is less than that of periodic motion of the orbiting electrons [3,4] i.e. $t = \frac{2\pi n^3}{Z^2} 2.42 \times 10^{-17}$ sec., where n and Z is the principle quantum number of concerned shell and the atomic number of the corresponding atomic system, respectively. The condition of suddenness of the perturbation can be satisfied during various nuclear processes (central nuclear potential change), for example, β-decay [5,6], positron decay [7–9], α-transfer reactions [10], orbital electron capture [11,12], internal conversion [13,14], as well as in the several atomic processes (sudden alteration in the electronic configuration) e.g. photoionization [15], inner-shell ionization [16,17] etc. It has been reported that recoil of the atomic system during the radioactive decay process [6,18] and influence of external agents [4,19] can also lead to the ionization or excitation of the electrons. In a similar note, interestingly, during the swift heavy ion-atom close collisions (lower impact parameter), target or projectile nucleus receives a sudden gain of nuclear recoil which creates a sudden perturbation in the stable electronic configuration, and this subsequently initiates the shaking processes.

Using nonrelativistic hydrogenic wave functions, the basic calculation of shaking probability due to the sudden jolt of the nucleus of the hydrogen atom has been reported in various texts [20,21]. In the earlier theoretical study [22], we have extended the work [20,21] to determine the general analytical expressions for shaking probability for $K-$, $L-$ and $M-$shell electrons of the hydrogen-like atomic systems. Whereas, in the present work, the previous study [22] has been further extended to define the generalized analytical expressions for survival and shakeup/shakedown probability for various subshells in any hydrogen-like atomic system. These expressions can be used to calculate the shaking and shakeup/shakedown probability in both the multielectron as well as the hydrogen-like atomic system during the swift heavy ion-atom collisions. Moreover, a thorough discussion emphasizing the recoil effects on the shaking process is presented.

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2. Shaking process

The shaking process can be realized as a two-step process, wherein the first step, due to the sudden perturbation, the central potential and/or electronic environment of the atomic system gets disturbed. In the case of swift heavy ion-atom collisions, this step corresponds to the sudden impact of projectile and target nucleus. Noteworthy that the condition of suddenness of the impact can be realised as the short Coulomb interaction ($\tau \ll t$) at nucleus-nucleus distances close to the perihelion compare to orbital motion of the electrons. The time period of this perturbation can be given by [4]

$$\tau = \frac{2d}{v}\left(1 + \sqrt{1 + \frac{b^2}{d^2}}\right) \tag{1}$$

here, v, d and b are the projectile velocity, closest approach and impact parameter, respectively.

Whereas, in the second step as a consequence of such perturbation, electrons make the transition to a new state (shakeup/shakedown) or a continuum state (shakeoff). Worth mentioning that shaking due to the sudden jolt of nucleus strongly depends on the first step i.e. the amplitude of ion-atom impact. On the contrary in other processes, for example, orbital electron capture [11,12], inner shell ionization [16,17], etc., shaking does not depend on the physical nature of the first step.

The transition probability of the system from one state to another state is determined by the general quantum mechanics rules and expressed as the overlap integral of the corresponding wave functions [20,23]

$$W_{fi} = \left|\int \psi_f^* \psi_i^{(0)} dV\right|^2 \tag{2}$$

here, $\psi_i^{(0)}$ and ψ_f are the initial and final wavefunctions of the atomic system, respectively. For the typical case of hydrogen-like atomic systems, Eq. (2) can be rewritten as

$$W_{fi} = \left|\int \psi_{n'l'm'}^* \psi_{nlm} dV\right|^2 \tag{3}$$

here ψ_{nlm} and $\psi_{n'l'm'}$ are the non-relativistic hydrogenic wavefunction of the initial and final state of the atomic system, respectively, whereas n, l, m belong to different quantum numbers which have their usual meaning. In general, the shaking processes due to potential change favour the monopole transitions i.e. transitions in which the principal quantum number (n) of the final state is different from the initial state ($n' \neq n$) and all other quantum numbers remain same, i.e., $l' = l$ and $m' = m$. On the contrary, in the recoil case, shaking processes have contributions from various multipole terms also i.e. dipole, quadrupole, etc. [22]. Although, the dominant contributions to the shaking processes are from the monopole and dipole terms, whereas higher order terms less contribute in the shaking processes. Thus in a good approximation, one can neglect the quadrupole and onwards higher order multipole terms [18]. In the shakeoff probability calculation where a large number of transition states are required, one can use these approximations to simplify the calculations [6,18]. However, in the present work, analytical expressions for the shaking probability are determined without taking any approximation.

3. Theoretical work, results, and discussion

Let us assume that in the initial state, the rest lab frame of the respective nucleus is S, whereas in the final state or after the recoil, the moving frame is S'. In the sudden approximation limit, orbiting electrons can be viewed as frozen and thus the coordinates of associated electrons with the moving nucleus in the frame S' remain same as frame S. In the new Hamiltonian state, the wave function (ψ_f) of the electron in the frame S' is given by

$$\psi_f = \psi_i \exp\left(-i\vec{q}\,.\sum_k \vec{r}_k\right) \tag{4}$$

here, operator $\exp\left(-i\vec{q}\,.\sum_k \vec{r}_k\right)$ is defined as the translation operator associated with the moving frame of reference S'. The summation is over all Z electrons in the atomic system, ψ_i is the wave function of the electron in initial rest state of the corresponding atomic system and q being the wave vector of the final system which is given by

$$q = \frac{m_e}{M + Zm_e}\frac{p}{\hbar} \tag{5}$$

here, $p(=\sqrt{2E_R M})$ is the momentum of the recoiled nucleus with E_R recoil energy. Whereas M and Z are the atomic mass and atomic number, respectively and m_e is the electron mass. Worth mentioning that after the sudden perturbation, each electron has three possibilities in the final state of the atomic system. It may remain either in the same initial state or can make a transition to unoccupied bound state (shakeup/shakedown) or gets ionized to the continuum state (shakeoff). Thus, the total shaking probability can be computed by subtracting the survival probability i.e. the probability for all the electrons to remain in their initial state, from the total probability i.e. unity, as done by the earlier workers [24,25]. Accordingly, from Eqs. (3) and (4), for hydrogen-like atomic system, the shaking probability can be given by

$$W_{shaking} = 1 - W_S \tag{6}$$

here, $W_S = \left(\left|\int \psi_{nlm}^* \exp(-i\vec{q}\,.\,\vec{r})\, \psi_{nlm}\, dV\right|^2\right)$, is the survival probability [22].

In the case of multielectron atomic system, many transitions which correspond to the already filled states are forbidden due to Pauli exclusion principle. Thus, for multielectron atomic system, after including the corrections for the contributions to occupied states, the shaking probability can be given by

$$W_{shaking} = 1 - (W_S)^N - W_F \tag{7}$$

here, N represents the number of electrons present in the respective shell, whereas, W_F is the electron transition probability to filled bound states (from $n' = 1$ to x) and defined as

$$W_F = T\,(W_F^{n'l'm}) = \sum_{n'=1}^{n'=x}\sum_{l'=0}^{l'=x-1} T\left|\int \psi_{n'l'm}^* \exp(-i\vec{q}\cdot\vec{r})\, \psi_{nlm}\, dV\right|^2 \tag{8}$$

here, $n' \neq n$, $l' \neq l$ and T is the number of electrons present in $n'l'm$ shell of the respective atomic system. Noteworthy that for the case of electron transitions to empty bound states, W_F can be stated as shakeup/shakedown probability.

Using the non-relativistic hydrogenic wavefunctions [26], the analytical expressions for survival and shakeup/shakedown probability are calculated for different electronic subshells and the results are shown in Table 1.

For the typical case of the recoiling nucleus of the multielectron atomic system i.e. $^{63}Cu^+$ ion, shaking probability with respect to reduced wave vector ($P = a\,q/Z$, here $a = $ Bohr radius) and recoil energy (E_R) are calculated using the Eq. (7) and analytical expressions, shown in Table 1. The results are presented in the Figs. 1 and 2. In the limiting condition, it is found that for the values of $P \ll 1$, shaking probability reduces to zero (for $P < 1$, $W_{shaking} \propto P^2$) whereas for $P \gg 1$ it tends to unity. The

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