Model for x-ray energy shifts for additional atomic vacancies

J. Bhattacharya, U. Laha, and B. Talukdar
Department of Physics, Visva-Bharati University, Santiniketan-731 235, West Bengal, India
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By using analytical self-consistent field functions in the model of Burch *et al.*, we have constructed an exact analytical expression for the K-shell x-ray energy shifts for an additional $2p$ vacancy. The expression is used to judge the quality of the model.

Heavy-ion collision experiments produce multiply ionized atoms with simultaneous vacancies in the inner and outer shells. The outer vacancies affect the energies of the diagram lines associated with the dominant mode of de-excitation of atom. Sometimes, one also observes nondiagram lines. Traditionally, the modification or change in the spectrum is interpreted in terms of the average energy of the singly ionized and multiply ionized configurations of the atom.[1,2] In this approach the actual number of computations involved is quite large. Burch *et al.*[3] have introduced a simple model for calculating the K-shell x-ray energy shift for an additional $2p$ vacancy. This model assumes that for all practical purposes the $2p$ vacancy may be treated as "permanent" in view of its relatively long lifetime compared with that in the K shell. The so-called permanent vacancy produces a change in the electrostatic potential experienced by the inner electrons and thereby causes shifts in the energy levels which are in turn reflected in the x-ray transition energies.

Two important extensions of this model have recently been made. For example, Roy *et al.*[4] extended it to arbitrary defect configurations while Bhattacharya *et al.*[5] incorporated the effects of relativity into the original model of Burch *et al.*[3] In these exploratory works the authors worked within the framework of a screened hydrogenic model and tried to gain some physical weight for the modification or change in the spectrum by different choices of the screening constants. Ideally, however, one would like to work with the self-consistent field functions and judge the quality of the model. The present paper is an effort in this direction.

According to Burch *et al.*,[3] a vacancy in the $2p$ shell produces a perturbing potential (in atomic units)

$$V_{2p}(r)=r^{-1}-r^{-1}\int_r^{\infty}P_{2p}(r')(r'^2-rr')dr' , \tag{1}$$

where $P_{2p}(r')$ is the charge density of the $2p$ electrons. The $2p$ energy shifts for the $K\alpha$ and $K\beta$ x rays are given by

$$\Delta K\alpha=(\Delta E)_{1s}-(\Delta E)_{2p}$$

and (2)

$$\Delta K\beta=(\Delta E)_{1s}-(\Delta E)_{3p} ,$$

where the binding energy shift $(\Delta E)_t=\langle t \mid V_{2p} \mid t \rangle$ with $t=1s$, $2p$, and $3p$, respectively. We have calculated $(\Delta E)_t$ by using self-consistent field functions in which occupied orbitals are expanded in terms of nodeless Slater-type functions according to

$$\phi_i=\sum_j C_{ij}[(2n_{ij})!]^{-1/2}(2\rho_{ij})^{[n_{ij}+(1/2)]}r^{n_{ij}}e^{-\rho_{ij}r} . \tag{3}$$

Here i labels the occupied orbitals and j the basis functions. The expression for $(\Delta E)_t$ is obtained as

$$(\Delta E)_t=\sum_{j_1j_2}C_{tj_1}C_{tj_2}[(2n_{tj_1})!]^{-1/2}[(2n_{tj_2})!]^{-1/2}(2\rho_{tj_1})^{[n_{tj_1}+(1/2)]}(2\rho_{tj_2})^{[n_{tj_2}+(1/2)]}$$
$$\times\left[\frac{\Gamma(n_{tj_1}+n_{tj_2})}{(\rho_{tj_1}+\rho_{tj_2})^{(n_{tj_1}+n_{tj_2})}}-\sum_{j_1'j_2'}C_{2pj_1'}C_{2pj_2'}[(2n_{2pj_1'})!]^{-1/2}[(2n_{2pj_2'})!]^{-1/2}(2\rho_{2pj_1'})^{[n_{2pj_1'}+(1/2)]}\right.$$
$$\times(2\rho_{2pj_2'})^{[n_{2pj_2'}+(1/2)]}\left[\frac{\rho_{tj_1}+\rho_{tj_2}+\rho_{2pj_1'}+\rho_{2pj_2'}}{\rho_{2pj_1'}+\rho_{2pj_2'}}\right]^{(n_{2pj_1'}+n_{2pj_2'})}$$
$$\left.\times\frac{\Gamma(n_{tj_1}+n_{tj_2}+n_{2pj_1'}+n_{2pj_2'}+1)}{(\rho_{tj_1}+\rho_{tj_2}+\rho_{2pj_1'}+\rho_{2pj_2'})^{(n_{tj_1}+n_{tj_2}+n_{2pj_1'}+n_{2pj_2'})}}\right]$$

$$\times\left[\frac{(\rho_{tj_1}+\rho_{tj_2}+\rho_{2pj'_1}+\rho_{2pj'_2})}{(n_{tj_1}+n_{tj_2})(\rho_{2pj'_1}+\rho_{2pj'_2})}\,{}_2F_1(n_{tj_1}+n_{tj_2},-n_{2pj'_1}-n_{2pj'_2};n_{tj_1}+n_{tj_2}+1;A_t)\right.$$

$$\left.-\frac{1}{(n_{tj_1}+n_{tj_2}+1)}\,{}_2F_1(n_{tj_1}+n_{tj_2}+1,-n_{2pj'_1}-n_{2pj'_2}+1;n_{tj_1}+n_{tj_2}+2;A_t)\right], \tag{4}$$

with

$$A_t=\frac{\rho_{tj_1}+\rho_{tj_2}}{\rho_{tj_1}+\rho_{tj_2}+\rho_{2pj'_1}+\rho_{2pj'_2}}\ . \tag{5}$$

In deriving Eq. (4) we have used[6,7] the following equations:

$$\int_u^\infty x^{\nu-1}e^{-\mu x}dx=\mu^{-\nu}\Gamma(\nu,\mu u),\quad u>0,\quad \mathrm{Re}\mu>0 \tag{6}$$

$$\int_0^\infty x^{\mu-1}e^{-\beta x}\Gamma(\nu,ax)dx=\frac{a^\nu\Gamma(\mu+\nu)}{\mu(a+\beta)^{\mu+\nu}}\,{}_2F_1\left[1,\mu+\nu;\mu+1;1-\frac{a}{a+\beta}\right],$$

$$\mathrm{Re}(a+\beta)>0,\quad \mathrm{Re}\beta>0,\quad \mathrm{Re}(\mu+\nu)>0 \tag{7}$$

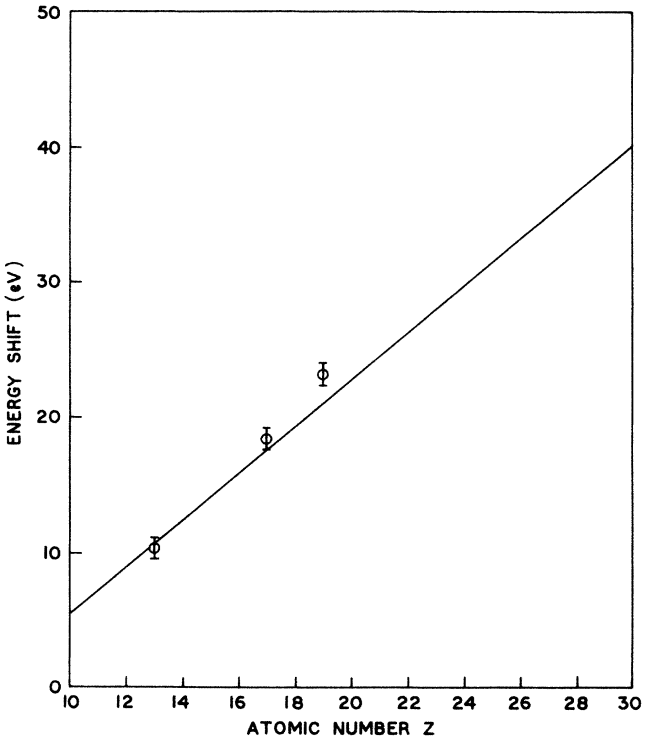

FIG. 1. $K\alpha$ x-ray energy shifts in eV as a function of Z, due to a missing $2p$ electron. Experimental results of Watson *et al.* have been denoted by Φ.

and

$${}_2F_1(a,b;c;Z)=(1-z)^{c-a-b}\,{}_2F_1(c-a,c-b;c;Z)\ . \tag{8}$$

The ${}_2F_1(\cdot)$ functions which occur in Eq. (4) are all polynomials since for nonrelativistic Hartree-Fock wave functions, $n_{ij}s$ are integers. Therefore our expression for $(\Delta E)_t$ is expected to give the best numerical result within the framework of the chosen model.

Weber *et al.*[8] have obtained Slater-type orbitals (STO's) of the form (3) for the neon atom by using the Fock-type operator which varies between the Hartree and Hartree-Fock operator and depends on a cutoff parameter r_{12}^0 in the exchange potential. The parameters of the STO's have been tabulated for selected values of r_{12}^0. The Hartree wave functions correspond to $r_{12}^0=0$ while the full Hartree-Fock values are for $r_{12}^0=\infty$. We have chosen to work with the wave functions of Weber *et al.* to compute the x-ray energy shifts of ${}_{10}$Ne by employing the results in Eq. (4).

For the Hartree and Hartree-Fock wave functions we obtained $\Delta K\alpha=5.8$ and 5.6 eV, respectively. We have verified that the Hartree-Fock wave functions of Clementi *et al.*[9] also give $\Delta K\alpha=5.6$ eV. Bhalla and Hein[10] have calculated the value of $\Delta K\alpha$ for ${}_{10}$Ne in terms of the average energies of singly and doubly ionized configurations. By using numerical Hartree-Fock wave functions they found $\Delta K\alpha=5.2$ eV. This number compares quite well with our Hartree-Fock result. One would, however, like to see whether the model is still good for other elements. Keeping this in view we have computed values for $\Delta K\alpha$ for elements from $Z=22-30$ by using the Hartree-Fock-Slater wave functions of Watson.[11] The results for $\Delta K\alpha$ as a function of Z are shown in Fig. 1. The Z dependence of the energy shifts is observed to be linear and the straight line obtained by us fits the data for ${}_{10}$Ne. In this figure we have also included the experimental values[12] for ${}_{13}$Al, ${}_{17}$Cl, and ${}_{19}$K. Interestingly, our curve (straight line) fairly interpolates these experimental values. Thus the simple-minded model of Burch *et al.*[3] seems to be quite reliable for quantitative estimates of the $K\alpha$ x-ray energy shift due to an additional vacancy in the $2p$ shell. As for the $K\beta$ x-ray energy shift due to a $2p$ vacancy we have computed $\Delta K\beta$ for ${}_{29}$Cu and found $\Delta K\beta=106.21$ eV. This result compares quite well with the experimental value (100 eV) of Rinsvelt *et al.*[13]

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