PHYSICAL REVIEW A VOLUME 38, NUMBER 7 OCTOBER 1, 1988

Green's-function calculation of the Auger energy

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(Received 4 February 1988)

Using the Green's-function method, the $M_5-N_{23}N_{45}$ Auger energy of the atomic Xe ($Z=54$) is calculated. In contrast to the Dirac-Hartree-Fock self-consistent-field (ΔSCF) method, which gives very poor agreement with the experiment both in absolute Auger energies and multiplet splitting energies, the present theory gives a good agreement with the experiment. The importance of the configuration interaction between the final double-hole level with the triple-hole one-electron continuum is pointed out as a cause of the large discrepancies between the ΔSCF results and experiment.

I. INTRODUCTION

Not only single electronic vacancy but also multiple electronic vacancies are often created in a gas of atoms or molecules or a solid surface by beams of photon or charged particles. Multiple holes are created by ionization or secondary emission precesses where a core hole cascades up towards the Fermi level and causes further ejections of electrons and photons. The observed electron and photon spectra provide information about the dynamics of the multiple holes created: relaxation shifts of the multiple hole levels, screening of the hole-hole Coulomb interactions and atom-solid, atom-molecule energy shift, and bulk-surface energy shift.

However, so far, in contrast to the case of a single-hole excitation, much less attention has been paid to the study of dynamics of multiple vacancies created in atomic like systems. Auger electron spectroscopy (AES) is one of the useful methods to study the electronic structures, particularly the dynamics of two holes created as the final state of the Auger decay process. In general the Auger energy can be well accounted for by calculating the difference of the total energy of the initial and final hole states within the framework of the Dirac-Hartree-Fock (DHF) self-consistent-field (ΔSCF) method and calculating the multiplet splitting in the intermediate coupling (IC) scheme. Some discrepancies in multiplet splitting and absolute energies remain irreducible even when configuration interaction (CI) is included both in the initial and final states of the Auger transition. The correlation effects in the final two-hole states are not only determined by CI and ground-state correlation (GSC) in the final ionic state of the Auger transition but also by (super) Coster-Kronig (SCK) fluctuations and decay processes in the final ionic state.

The analysis of the L_{23}-*MM* (except $M_{45}M_{45}$) Auger electron spectra of Zn and surrounding elements show that not only CI and GSC but also *MM-MMM* (SCK) fluctuation and decay processes in the final ionic state of the Auger transition have to be taken account to get better agreement with experiment.[1] The relaxation shifts due to CI between the two-hole final state and triple-hole continua are multiplet level dependent: These relaxation processes are effective not only in shifting the average Auger energy but also in screening the Coulomb hole-hole repulsion interaction which affects the term splitting.[1]

Another example of such behavior is found in the M_{45}-$N_{23}N_{45}$ Auger spectra of the elements Ag ($Z=47$) to Xe ($Z=54$).[2-4] The very broad M_{45}-$N_{23}N_{45}$ Auger spectra of the metallic elements in the range of Pd to Te arise from complete breakdown of the quasiparticle picture of the final-state double vacancy due to $4p^{-1}4d^{-1}\leftrightarrow 4d^{-3}\epsilon f$ (super) Coster-Kronig fluctuation and decay processes.[2,3] The M_{45}-$N_{23}N_{45}$ Auger spectrum of Xe shows a discrete structure; however the spectrum can not be interpreted within an atomic one-electronic picture. Aksela *et al.*[4] pointed out that the major features of the spectrum can be predicted by calculating the relative Auger energies (multiplet splittings) and intensities of the line components using the mixed coupling scheme applying *j-j* coupling for the initial state and intermediate coupling for the final state. They concluded that the shifts and line broadenings of the photoelectron spectrum (4*p* x-ray photoelectron spectroscopy spectrum) are not apparent in the Auger spectrum. However, they did not calculate the absolute Auger energies. As shown in the present work, the spectrum is shifted as much as ~18 eV from the DHF ΔSCF Auger energy and different multiplet lines have different energy shifts. This shows that it is very important to treat the correlations of the final double-hole in a proper way.

One of the systematic ways to describe the Auger spectrum is the two-hole Green's-function method. The Green's-function method was used a decade ago by Wendin and Ohno[5,6] in order to calculate the double-hole and multiple vacancy energies in terms of the screened hole-hole repulsion based on the knowledge of a single-hole relaxation shift and of the bare hole-hole Coulomb repulsion from the no-hole ground-state configuration. They extended the two-hole Green's-function method to calculate the double-hole spectral function in order to describe the Auger spectrum which is entirely governed by the dynamics of the final-state double holes.[2,3]

Recently Cederbaum[7] made a detailed study of the multiple hole spectrum by using the Green's-function method. The diagrammatic expansion of the double holes is similar to that considered previously by Wendin and Ohno.[5]

In the present work I use the Green's-function method to calculate the M_5-$M_{23}N_{45}$ Auger transition energies of Xe which are influenced very much by CI between the two-hole final state and triple hole-one particle state.

The Auger energies and multiplet splittings calculated by the Green's-function method give much better agreement with the experiment than the ones by the Dirac-hartree-Fock ΔSCF method, which give very poor agreement with the experiment.

II. THEORY

When the final two-hole states are assumed to be sharp and structureless (no broadening, no satellite structure), a one-step treatment of the photoionization-Auger emission process gives for Auger current[8]

$$I_A(\varepsilon;\omega) \sim \sum_i \int dE \, | \langle i \,|\, Z \,|\, E+\omega \rangle |^2 A_i(E) \times \sum_{j,k} \sum_{S,L} \frac{\pi \, | V^{SL}_{i\epsilon jk}(E) |^2}{\mathrm{Im}\Sigma_i(E)} \delta(\varepsilon - E^{SL}_{jk} + E) \,, \tag{1}$$

where ε is the Auger energy, ω is the photon energy, Z the dipole operator, E is the energy of the initial hole, (j,k) is the final two-hole state with spin S and orbital angular momentum L, and $A_i(E)$ is the spectral function of the initial hole i, given by

$$\begin{aligned} A_i(E) &= \frac{1}{\pi} \mathrm{Im} G_i(E) \\ &= \frac{1}{\pi} \frac{\mathrm{Im}\Sigma_i(E)}{[E - E^0_i - Re\Sigma_i(E)]^2 + [\mathrm{Im}\Sigma_i(E)]^2} \end{aligned} \tag{2}$$

where E^0_i is a relativistic Hartree-Fock Koopmans's energy. The self-energy $\Sigma_i(E)$ of the initial hole i is given by

$$\Sigma_i(E) = \sum_{j,k} \sum_{S,L} \int d\epsilon \frac{| V^{SL}_{i\epsilon jk}(E) |^2}{\epsilon - E^{SL}_{jk} + E - i\delta} \,, \tag{3}$$

where $V^{SL}_{i\epsilon jk}(E)$ is the excitation matrix element which accounts for the polarization, relaxation, and GSC effects involved in the excitation process:

$$V^{SL}_{i\epsilon jk} = \langle jk(SL) \,|\, 1/\gamma_{12} \,|\, i\varepsilon \rangle \,. \tag{4}$$

When the final-hole states are not sharp, we must consider a two-hole spectral function $A_{jk}(E)$ describing the interacting final hole states, i.e., not only the final ionic state interchannel interaction but also the configuration interaction between the final two-hole discrete and triple-hole one-electron continua. The Auger emission current is then

$$I_A(\varepsilon;\omega) \sim \sum_i \int dE \, | \langle i \,|\, Z \,|\, E+\omega \rangle |^2 A_i(E) \times \sum_{j,k} \sum_{S,L} \frac{\pi \, | V^{SL}_{i\epsilon jk}(E) |^2}{\mathrm{Im}\Sigma_i(E)} A^{SL}_{jk}(E+\omega) \,, \tag{5}$$

$$A^{SL}_{jk}(E+\omega) = \frac{1}{\pi} \mathrm{Im} G^{SL}_{jk}(E+\omega) \,. \tag{6}$$

Here $G^{SL}_{jk}(E)$ is the Green's function for the final double-hole j and k. The Green's function of the double hole X and Y is given by

$$G^{SL}_{XY}(E) = [E - (\varepsilon_x + \varepsilon_y) + F^0(X,Y) - \Sigma_{XY}(E) - \Delta^{SL}(X,Y)]^{-1} \,. \tag{7}$$

Here ε_x and ε_y are the unperturbed (Koopmans) single-hole energy of the hole X and Y, respectively. $F^0(X,Y)$ is the bare Coulomb hole-hole repulsion interaction and $\Delta^{SL}(X,Y)$ is the contribution for the multiplet splittings. Within the Hartree-Fock (HF) ΔSCF approximation, the self-energy of the double hole $\Sigma_{XY}(E)$ is approximated as follows:

$$\begin{aligned} \Sigma_{XY}(E) = \sum_{\substack{q\neq j \\ j\neq X,Y}} & \left[\frac{| \langle jX \| qX \rangle |^2}{\varepsilon_q - \varepsilon_j - \varepsilon_x - \varepsilon_y + E - i\delta} + \frac{| \langle jY \| qY \rangle |^2}{\varepsilon_q - \varepsilon_j - \varepsilon_x - \varepsilon_y + E - i\delta} \right] \\ & + 2 \sum_{\substack{q\neq j \\ j\neq X,Y}} \frac{\langle jX \| qX \rangle \langle qY \| jY \rangle}{\varepsilon_q - \varepsilon_j - \varepsilon_x - \varepsilon_y + E - i\delta} \,. \end{aligned} \tag{8}$$

Here $\langle p \| q \rangle$ denotes

$$\langle p(2) \| q(2) \rangle r(1) = \int d\tau_2 P^*(2) \frac{1}{r_{12}} [q(2)r(1) - r(2)q(1)] \tag{9}$$

and j is the occupied (hole) level. q is the unoccupied (particle) level. The first two terms describe the relaxation in the presence of a single hole X and Y, respectively: the nonhole hopping (mainly monopole) relaxation. The second term describes the screening of the bare Coulomb hole-hole repulsion interaction. Within the second-order Hartree-Fock approximation the self-energy is given by

$$\Sigma_{XY}(E) = \sum_{i=X,Y} [\Delta^R_i(E)] + \sum_{i=X,Y} [\Delta^C_i(E)] + 2\Delta^{SC}_{XY}(E) + \Delta^C_{XY}(E) + F^{(1)}_{XY}(E) \,. \tag{10}$$

Here

$$\Delta^R_X(E) = \sum_{i,j,a} \frac{| \langle ij \| aX \rangle |^2}{E + \varepsilon_a - \varepsilon_i - \varepsilon_j - \varepsilon_y - i\delta} \,, \tag{11a}$$

$$\Delta^C_X(E) = \sum_{i,a,b} \frac{| \langle ab \| Xi \rangle |^2}{E + \varepsilon_i - \varepsilon_a - \varepsilon_b - \varepsilon_y - i\delta} \,, \tag{11b}$$

$$\Delta^{SC}_{XY}(E) = \sum_{g,j} \frac{\langle jX \| qX \rangle \langle qY \| jY \rangle}{\varepsilon_q - \varepsilon_j - \varepsilon_x - \varepsilon_y + E - i\delta} \,, \tag{11c}$$

$$\Delta_{XY}^{C}(E)=\sum_{a,b}\frac{|\langle XY\|ab\rangle|^{2}}{E-\varepsilon_a-\varepsilon_b-i\delta}\ , \tag{11d}$$

$$F_{XY}^{1}(E)=\sum_{i,j}\frac{|\langle ij\|XY\rangle|^{2}}{E-\varepsilon_i-\varepsilon_j-i\delta}\ , \tag{11e}$$

where i and j are the occupied levels and a and b are the unoccupied levels. The first term is the relaxation term of a single hole. We note that the relaxation term now includes the hole-hopping terms, in contrast to the case when we work only within the framework of ΔSCF picture. The hole-hopping terms are often dominated by (super) Coster-Kronig processes. The second term is the ground-state correlation term of a single hole. The third term is the screening of the bare Coulomb hole-hole repulsion interaction. The fourth term describes the pair ground-state correlation energy of the double hole X and Y. The last term is the second-order term with respect to the bare hole-hole Coulomb interaction (including the nondiagonal hole-hopping interaction). When the holes are created in the same atomic shell ($X=Y$), Eq. (10) becomes much simpler:

$$\begin{aligned}\Sigma_{XX}(E)={}&2\Delta_X^{R}(E)+2\Delta_X^{C}(E)+2\Delta_{XX}^{SC}(E)\\&+\Delta_{XX}^{C}(E)+F^{(1)}(X,X)\ .\end{aligned} \tag{12}$$

The Green's function of the double hole X is given now by

$$G_{XX}^{SL}(E)=[E-2\varepsilon_x+F^{0}(X,X)-\Delta^{SL}(X,X)-\Sigma_{XX}(E)]^{-1}\ . \tag{13}$$

As in the case of a single-hole Green's function it is often numerically expensive to evaluate the all diagrams for the self-energy. Then it is much more economical to evaluate an infinite sum of the certain diagrams by the HF ΔSCF method. Then the double-hole Green's function becomes

$$G_{XY}^{SL}=[E-E_{XY}^{SL}(\Delta\mathrm{SCF})-\Sigma_{XY}(E)]^{-1}\ , \tag{14}$$

$$\begin{aligned}\Sigma_{XY}(E)={}&\Delta_X^{DR}(E)+\Delta_Y^{DR}(E)+\Delta_X^{C}(E)+\Delta_Y^{C}(E)\\&+\Delta_{XY}^{C}(E)+F_{XY}^{(1)}(E)+2\Delta_{XY}^{SL}(E)\ .\end{aligned} \tag{15}$$

Here $E_{XY}^{SL}(\Delta\mathrm{SCF})$ energy for the double hole X and Y coupled to the specified angular momentum and spin state LS. Here $\Delta_X^{DR}(E)$ is the hole-hopping (dipole fluctuation) relaxation terms of the single hole X.

$\Delta_{XY}^{SC}(E)$ now includes only the nondiagonal part (dipole screening term). Now we consider the renormalization of the second-order self-energy which is given by the following general expression:

$$\Sigma_i(E)=\sum_{m,j,k,l}\frac{V_{jkim}V_{imjk}}{E_m^0-E_j^0-E_k^0-E_l^0+E-i\delta}\ , \tag{16a}$$

$$V_{jkim}=\langle jk\ |\ 1/V_{12}\ |\ im\rangle\ . \tag{16b}$$

We consider the renormalization of the self-energy by approximating the effective four-body [one particle (p), three holes (h) phhh] interaction $I^{\mathrm{phhh}}(E)$ by the sum of the effective two-body interactions $I^{\mathrm{ph}}(E)$ and $I^{\mathrm{hh}}(E)$. The true four-body part $I^{\mathrm{phhh}}(E)$ only represents a small higher-order correction and may be neglected. The self-energy can be renormalized by introducing the effective hole-hole interaction $I^{\mathrm{hh}}(E)$ to the intermediate holes j, k, and l:

$$E_j^0+E_k^0+E_l^0\rightarrow E_{jkl}(E)\ , \tag{17a}$$

$$\begin{aligned}E_{jkl}(E)={}&E_j(E)+E_k(E)+E_l(E)-I_{jk}^{\mathrm{hh}}(E)\\&-I_{kl}^{hh}(E)-I_{jl}^{\mathrm{hh}}(E)\ .\end{aligned} \tag{17b}$$

The self-energy can be renormalized further by including the effective particle-hole interaction $I^{\mathrm{ph}}(E)$. The self-energy is now obtained in the form

$$\Sigma_i(E)=\sum_{m,j,k,l}\frac{V_{jkim}\Gamma_{imjk}(E)}{E_m^0-E_{jkl}(E)+E-i\delta}\ . \tag{18}$$

With the effective interaction $\Gamma_{imjk}(E)$ given by a Bethe-Salpeter integral equation,

$$\Gamma_{imjk}(E)=V_{imjk}+\sum_{m'}\frac{[I^{\mathrm{ph}}_{jmjm'}(E)+I^{\mathrm{ph}}_{kmkm'}(E)+I^{\mathrm{ph}}_{lmlm'}(E)]\Gamma_{im'jk}(E)}{E_{m'}^0-E_{jkl}(E)+E-i\delta}\ . \tag{19}$$

In the present work we evaluate the self-energy using an extended version of the renormalized second-order expressions Eqs. (18) and (19),

$$\Sigma_i(E)=\sum_{m,j,k,l}\frac{U_{jkim}\Gamma_{imjk}(E)}{E_m^0-E_{jkl}(E)+E-i\delta}\ , \tag{20}$$

$$\Gamma_{imjk}(E)=U_{imjk}+\sum_{m'}\frac{[I^{\mathrm{ph}}_{jmjm'}(E)+I^{\mathrm{ph}}_{kmkm'}(E)+I^{\mathrm{ph}}_{lmlm'}(E)]\Gamma_{im'jk}(E)}{E_{m'}^0-E_{jkl}(E)+E-i\delta}\ , \tag{21}$$

$$U_{imjk}=V_{imjk}-\sum_{m',k'}\frac{V_{im'jk'}V^{gsc}_{m'mk'k}}{E_m^0-E_k^0+E_{m'}^0-E_{k'}^0}\ , \tag{22}$$

where we note that we replaced V_{imjk} by U_{imjk}, which includes the time reversed diagrams describing Fermi-sea correlation effects. Here V^{gsc} is the interaction matrix element to describe Fermi-sea correlations. (See diagram (h) in Fig. 5 in Ref. 5. In the present case one has to add an extra $4d$ hole propagator to diagram (h).] We solve Eqs. (20) and (21) within the random-phase approximation with exchange.[5] In this approximation the screening of the electrostatic interaction between the particle and extra holes and relaxation of the excited electron is neglected. This approximation becomes questionable when the variation of the continuum density is rapid and it breaks down for low-lying localized ionic excitations. The screening of the hole-hole repulsion $I^{hh}(E)$ is calculated in the static monopole approximation and the triple-hole energy $E_{jkl}(E)$ is obtained by the Dirac-Hartree-Fock ΔSCF method.

III. EVALUATION OF THE GREEN'S FUNCTION

In the present work we use Eq. (14) and (15) for evaluation of the Green's function. We neglect the GSC contributions in the present work, because these contributions are small (at most order of 2 eV) and negligible for the present purpose of the calculations. The $4p^{-1}4d^{-1} \leftrightarrow 4d^{-3}n(\epsilon)f$ SCK process dominates the energy shift at the $4p^{-1}4d^{-1}$ level from the DHF ΔSCF energy. In the present work, as we are particularly interested in the energy shift beyond the HF ΔSCF picture, we consider only CK (SCK) processes when calculating the self-energy.

Basis sets: Zeroth-order basis set will be chosen as follows.

(i) For the hole (i,j,k,l) states: We use nonrelativistic HF orbitals of the neutral atom ground state.

(ii) For the particle (m) states: Three-hole (V^{N-3}) HF potential constructed by frozen ground state orbitals. The excited electron m is coupled to the core hole k to a ^1P total angular momentum state. The core holes j and l are spectators, contributing only to the spherically symmetric Hartree potential,

$$(j^{-1})_{\rm av}(l^{-1})_{\rm av}(k^{-1}m\ {}^1P)\text{HF } V^{N-3} \text{ potential .} \qquad (23)$$

Using this basis is the same as working in the Tamm-Dancoff approximation with exchange for the $k^{-1}m$ dipole response and including the Hartree potential from the second and third holes j and l. The Fermi sea correlation diagrams can now be expanded through the integral equation (21).

Energy parameters: We introduce the monopole relaxation energy shift (relaxation energy shift within the ΔSCF picture) and relativistic energy shifts in the energy parameters. However, the approximation is not fully consistent in the sense that the monopole relaxation and relativistic effects are included only in terms of the double-hole and triple-hole level shifts while the corresponding effects on the wave functions are neglected. The unperturbed initial double-hole energies E_{XY}^{SL}(ΔSCF (DHF ΔSCF energies) have been evaluated by the Dirac-Fock program of Grant *et al.*[9,10] using the intermediate coupling without the configuration interaction between the double-hole configurations. The triple-hole energy $E_{jkl}(E)$ has been also evaluated by the DHF ΔSCF method. In the case of triple-hole energy we neglect the multiplet splittings and use the average triple-hole DHF ΔSCF energy.

We first calculated the double-hole Green's function by using the self-energy for which the unoccupied orbitals are obtained by the V^{N-3} HF potential of triple-hole configuration so that one includes the effect on the virtual orbitals by the presence of three $4d$ holes. However, the results show that the relaxation energy shift is underestimated and the multiplet splitting is not well described. We calculated also by using the self-energy for which the unoccupied (virtual discrete and continuum) orbitals are generated by a V^{N-2} potential which neglects the presence of the third $4d$ hole. In the present work we discuss the results obtained by the latter method, which gives much better agreement with experiment.

IV. RESULTS AND DISCUSSION

Before I discuss the present theoretical results by comparing them with the experimental data, I should comment on the experimental data by Aksela *et al.*[4] They decomposed the M_{45}-$N_{23}N_{45}$ Auger spectrum of Xe, assuming that the one-electron picture and the multiplet splittings considered within the one-electron picture are valid. The spectrum consists of many low intensity lines which make it very difficult to decompose the spectrum in an accurate way.

As the present many-electron effects are considered to be independent of the initial $3d$ hole state, we expect the statistical ratio of 2:3 for the M_4-$N_{23}N_{45}$ to M_5-$N_{23}N_{45}$ Auger spectrum intensities. However, the experimental intensity ratio is 1:1. This implies that there is a possibility of errors occurring in the decomposition procedure of the spectrum.

Note that the lower energy side of the M_5-$N_{23}N_{45}$ Auger spectrum and the higher energy side of the M_4-$N_{23}N_{45}$ Auger spectrum are not influenced by the presence of other spectrum. Then the multiplet levels (first five multiplet levels) in the lower energy region can be determined accurately from the M_5-$N_{23}N_{45}$ Auger spectrum and the next four multiplet levels can be determined from the M_4-$N_{23}N_{45}$ Auger spectrum. As these multiplet levels of the M_5-$N_{23}N_{45}$ Auger spectrum overlap with the lower energy region of the M_4-$N_{23}N_{45}$ Auger spectrum, there is a large uncertainty in their intensities.

The last two or three multiplet levels of the M_5-$N_{23}N_{45}$ Auger spectrum fall into the large intensity region of the M_4-$N_{23}N_{45}$ Auger spectrum and the corresponding levels of the M_4-$N_{23}N_{45}$ Auger spectrum lie in the very low intensity region. This makes it very difficult to determine the positions and intensities of these levels.

Aksela *et al.*[4] calculated the intensities of the line components by the mixed coupling scheme applying *jj* coupling for the initial state and intermediate coupling for the final state. However, this kind of conventional scheme is not good enough in the present case because of

TABLE I. Experimental and theoretical (DHF ΔSCF) M_5-$N_{23}N_{45}$ Auger transition energies of Xe (in units of eV). The experimental data are from Ref. 4.

	Auger energy			Multiplet splitting		
Level	Expt.	DHF ΔSCF	Difference	Expt.	DHF ΔSCF	Difference
$^1F_3$	433.5	415.67	17.8	0.0	0.0	0.0
$^1P_1$	435.5	417.18	18.3	1.95	1.51	0.44
$^3P_2$	438.0	422.62	15.4	4.55	6.95	−2.40
$^3D_1$	440.7	425.52	15.2	7.15	9.85	−2.70
$^3D_3$	442.9	429.46	13.6	9.36	13.79	−4.43
$^3D_2$	444.2	431.1	13.1	10.66	15.43	−4.77
$^3P_0$	445.3	433.06	12.2	11.83	17.39	−5.56
$^3F_2$	445.3	433.26	12.0	11.83	17.59	−5.76
$^3F_3$	446.5	433.71	12.8	13.00	18.04	−5.04
$^3P_1$	449.5	436.69	12.8	16.02	21.02	−5.0
$^1D_2$	453.4	438.74	14.7	19.89	23.07	−3.18
$^3F_4$	454.4	440.94	13.5	20.93	25.27	−4.34

neglect of many-electron effects of the $4p4d$ double-hole state.

The validity of assignment of the lines of the spectrum according to the standard angular momentum coupling scheme requires discussion. In the present case the one-electron picture of the $4p4d$ double hole breaks down due to the strong CI between the $4p4d$ double-hole level and $4d^{-3}(n)\epsilon f$ excitations. This strong CI (super Coster-Kronig process) causes a splitting of the original $4p4d$ double-hole multiplet level into the split-off level and the nonresonant continuum. However, the present calculation shows that a large part (70–80%) of the original strength (which differs for different multiplet levels) goes to the split-off level which appears as the discrete structure of the M_{45}-$N_{23}N_{45}$ Auger spectrum. This split-off level originates from mixing of a discrete $4p4d$ double-hole level with a band of $4d^{-3}\epsilon f$ excitations. In this band the ϵf wave functions tend to localize resonantly in the region of the $4p$ and $4d$ orbitals, thereby acquiring collapsed $4f$-like character. As a large of the original angular momentum state exists in the split-off level, the assigned angular momentum state should be considered as the original state of the split-off level.

In Table I we list the M_5-$N_{23}N_{45}$ DHF ΔSCF Auger energies. In order to study only the correlation effects of the final $4p4d$ double-hole states, the experimental M_5 hole energy (676.7 eV) is used for both DHF ΔSCF and the present many-body calculations.

The experimental Auger energy is shifted as much as 18 eV from the DHF ΔSCF Auger energy. The energy shift from the DHF ΔSCF Auger energy differs for different multiplet terms. The multiplet splitting calculated by using the intermediate coupling differs very much from the experimental results. In Table II we list the Auger energies obtained by the present many-body calculation. One should note the following points.

(i) The present many-body calculation shows that the energy shifts of the $4p4d$ multiplet levels due to CI between the $4p4d$ two-hole and $4d$ triple-hole configurations result in the range of 8–16 eV.

(ii) The present calculation shows that the relaxation energy shifts of the $4p4d$ multiplet levels differ for different multiplet levels. This is because the dipolar fluctuation process which strongly shifts the $4p4d$ level is now also effective in screening the $G^1(4p,4d)$ integral which influences the term splitting in a quite important

TABLE II. Experimental and theoretical (present theory) M_5-$N_{23}N_{45}$ Auger transition energies of Xe (in units of eV). Experimental data are from Ref. 4.

	Auger energy			Multiplet splitting		
Level	Expt.	Theory	Difference	Expt.	Theory	Difference
$^1F_3$	433.5	431.4	2.1	0.0	0.0	0.0
$^1P_1$	435.5	432.2	3.3	1.95	0.8	1.15
$^3P_2$	438.0	435.5	2.5	4.55	4.1	0.45
$^3D_1$	440.7	437.5	3.2	7.15	6.1	1.05
$^3D_3$	442.9	440.2	2.7	9.36	8.8	0.56
$^3D_2$	444.2	441.5	2.7	10.66	10.1	0.56
$^3P_0$	445.3	443.0	2.3	11.83	11.6	0.23
$^3F_2$	445.3	443.1	2.2	11.83	11.7	0.13
$^3F_3$	446.5	443.5	3.0	13.00	12.1	0.9
$^3P_1$	449.5	445.8	3.7	16.02	14.4	1.62
$^1D_2$	453.4	447.4	6.0	19.89	16.0	3.89
$^3F_4$	454.4	449.3	5.1	20.93	17.9	3.03

way in contrast to the case of, e.g., a 4*d* double vacancy, where monopole relaxation is only effective in screening the average Coulomb interaction (F^0 integrals), which only affects the average Auger energy and the term splitting is changed very little. Note that the intermediate coupling scheme works quite well for the multiplet splitting of the M_{45}-$N_{45}N_{45}$ Auger transitions of Xe, in contrast to the case of the M_{45}-$N_{23}N_{45}$ Auger transitions.[4]

(iii) Even taking into account the uncertainties in the decomposition of the spectrum, the present result gives good agreement with experiment. Note that the deviation in the Auger energy between the present result and experiment is fairly constant and of the order of 2.5 eV, in contrast to the case of the DHF ΔSCF results, which deviate as much as 18 eV. In the case of multiplet splitting the deviation from the present result is at most 1 eV, in contrast to the DHF ΔSCF result, which deviate as much as 5–6 eV.

A relatively large deviation in both absolute and relative Auger energy for $^3P_1$, $^1D_2$, and $^3F_4$ levels could be due to errors occurred in the process of decomposing the Auger spectrum at the higher energy region. Judging from a good agreement with experiment in the lower Auger energy region where the decomposition of the spectrum is reliable, it is reasonable to conclude that the experimental intensity ratio of 1:1 of the M_4-$N_{23}N_{45}$ and M_5-$N_{23}N_{45}$ Auger transitions is most likely due to the errors in the determination of intensities in the higher energy region above 446 eV.

(iv) In the present work we neglected the effect of the presence of an extra hole on the virtual orbitals. When we include the effect of the presence of an extra hole on the virtual orbitals simply by taking a spherical average of the extra hole, the results are very poor. This implies that it is necessary to include the screening of the interaction between the extra hole and the virtual electron so that the effect of the presence of this extra electron on the virtual electron will be much more reduced.

V. CONCLUDING REMARKS

The present many-body calculation of the atomic Auger energy using the Green's-function method shows that it is fairly important to take into account the configuration interaction between the final-state double-hole levels and the triple-hole one-electron continuum when the one or both of the final-state double holes involves the strong dynamical relaxation processes. The dynamical screening of the Coulomb interaction between the final-state double hole also influences the multiplet splitting very much. In the present calculation the configuration interaction among the final ionic states is neglected. In general the energy shift due to such a configuration interaction is very small.

ACKNOWLEDGMENT

The author is very grateful to K. Ohno and S. J. Henke for support during the course of the present work.

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