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Xenon L emission spectra and many-electron effects in core levels

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Nine L x-ray emission lines of xenon ($Z=54$) in the gas phase were measured in fluorescence. The spectra were obtained on a double-crystal spectrometer using a conventional x-ray tube for primary excitation. The binding energies of the L subshells were obtained using the experimental x-ray photoelectron-spectroscopy (XPS) ionization energies of the final states and found to be in agreement with earlier XPS measurement. The K-shell binding energy was also determined. The transition energies, level energies, and widths were analyzed with respect to available experimental and theoretical data. Discrepancies between experiment and theory are discussed in terms of dynamical relaxation and decay. It is suggested that this discrepancy can be mended by using the many-body approach such as the Green's-function method, which treats such strong correlations in a consistent way.

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I. INTRODUCTION

X-ray emission spectroscopy (XES) provides useful information of the electronic structure of a system and the dynamic excitation processes involved. There are very few x-ray photoelectron-spectroscopy (XPS) measurements [1] having incident photons with higher energy than Al $K\alpha$ radiation. The measurement of XES in conjunction with available XPS measurements of the final states permits the extraction of information on the excited initial states beyond the limit Al $K\alpha$ radiation. An attractive group of atomic systems are the rare gases that are monoatomic at room temperature with ground-state closed-shell configurations. Their unique electronic structure and distribution in the Periodic Table have provided theoreticians with prime subjects to test and improve theory.

The precision measurement of the xenon L emission spectra has not been reported to our knowledge except for the report [2] of the $L\gamma_{2,3}$ spectral region. A low-resolution study of the Xe L spectra excited by electron impact that was recorded with a Si(Li) detector has been reported by Hippler *et al.* [3]. Their interest was to measure the ionization cross section of the L subshells of xenon by low-energy electron impact (6–14 keV). The L_1, L_2, and L_3 absorption edges of gaseous xenon were measured by Watanabe [4] with high resolution to obtain the jump ratios of the edges, the mass-absorption coefficients, and an estimate of the oscillator strengths for the bound state to bound state transitions. Breinig *et al.* [5] measured the x-ray absorption near-edge (XANE) regions of some rare gases including the L subshells of xenon. The L-subshell binding energies (BE's) were extracted by modeling the XANE structure. Complementing these works are the XPS measurements [6] of the electronic levels of xenon up to a BE of 1148.7 eV ($3s_{1/2}$) and the Auger-electron-spectroscopy (AES) work by a number of workers [7]. The precision measurement [8] of the $K\alpha_{1,2}$ and $K\beta_{1,3}$ line positions and widths of xenon were determined as a part of an experimental study of K lines of heavy elements.

The present paper will report on the high-resolution measurement of most of the xenon L spectral lines. The $L\gamma_{2,3}(2s^{-1}\text{-}4p^{-1})$ XES spectrum of Xe (and surrounding elements) [2,9–11] has been reported earlier. The $L\gamma_{2,3}$ spectrum was interpreted in terms of the spectral function of the final $4p$ hole and shows the breakdown of the quasiparticle picture of a $4p$ hole due to strong dynamical correlations [2,9–11]. In the present report we shall make an analysis of the energies and widths of the L x-ray emission spectra by using the available theoretical and experimental energies and widths of a single hole. A similar analysis was made of the L emission [12] of the elements $Z=41$ to 51 (Nb to Sb) and the $K\alpha$ and $K\beta$ emission [13] from $Z=42$ to 97 (Mo to Bk). We discuss the discrepancies between theory and experiment in terms of many-electron effects and point out that these discrepancies can be mended by many-body calculations from the theoretical side.

II. EXPERIMENT

The fluorescent xenon L XES spectra were measured on a vacuum double-crystal spectrometer [14] using high-quality Ge(220) crystals ($2d=4.000\,675\,4$ Å at 22.5 °C [15]. Commercial CP-grade xenon gas was contained in a fluorescence cell [16] by 25-μm-thick beryllium windows at a pressure of 0.13 kPa (100 Torr). A high-power x-ray tube with a cobalt-plated copper anode operating at 13 kV and 190 mA provided the primary exciting radiation. The monochromatized radiation from xenon was detected with a gas-flow proportional counter filled with P-10 gas (90% argon, 10% methane) at a pressure of 0.92 kPa (700 Torr). The spectra were obtained by scanning the second crystal in steps.

The procedure used to measure the spectra was to start about 1 h after the x-ray tube and necessary electronics had been operating at the measurement level. The spectrum of interest was always sandwiched between two diffraction profiles $(1,-1)$. All the measured spectral profiles were individually fitted [17] by least-squares modeling of the profiles with Voight functions and a linear background. The peak position of the two sandwiching diffraction profiles were averaged to provide the parallel $(1,-1)$ position in determining the Bragg angle of the dispersed $(1,1)$ spectrum between them. Thus all the spectral profiles were individually analyzed. Corrections for crystal temperature [$\alpha=5.95(11)\times10^{-6}$ K^{-1}] [15], vertical divergence, index of defraction δ/λ^2 of the Ge [18] ranging from 6.29 to 6.39×10^{-4} nm^2 and crystal angular reading were applied [19] to the fitted spectral-peak positions. The corrected individual Bragg angle of the peak positions were then averaged for each spectral line. Three to five sets of spectra were obtained for each spectral line. The total corrections applied ranged from 97 ppm for $L\gamma_1$ to 136 ppm for *Ll*. The uncertainties in the corrections are as follows:

Index of refraction	0.3 ppm
Vertical divergence	1.0
Temperature	1.0
Angle reading	2.0
Total	4.3 ppm

The conversion value of $V\lambda=1.239\,842\,44\times10^{-6}$ eV m from the 1986 adjustment [20] of fundamental constants is used in presenting the spectral data. The uncertainty of the experimental energy sale of ±0.04 eV is primarily due to counting statistics and modeling of the spectral lines. The diffraction rocking curve had a full width at half maximum (FWHM) that ranged from 0.26(2) to 0.50(3) eV.

III. RESULTS AND DISCUSSION

A. X-ray emission energies

In Table I we list the *L* x-ray emission energies measured in the present work and the x-ray emission energies obtained by using the experimental (XPS) single-hole ionization energies. The difference of less than 1.0 eV except for L_l indicates good agreement between the present x-ray emission data and XPS data. The Dirac-Hartree-Fock self-consistent-field (DHFΔ SCF) x-ray emission energies obtained by using the DHFΔSCF single-hole energies calculated by Beatham *et al.* [21] are tabulated also in Table I. Note that there is a significant discrepancy between experiment and DHFΔSCF results. We will discuss the origin of these discrepancies in the remaining portion of this section.

Strictly speaking, the Hartree-Fock orbital energies (Koopmans's approximation) have no physical relevance because of the neglect of ground-state and final-state correlation and relaxation in the final state. In order to calculate so-called Koopmans's defect, one may employ the perturbation expansion scheme. The perturbation expansion of the ionization energy in terms of the self-energy at the level of the second-order approximation shows already that the ionization energy shift beyond the Koopmans's approximation can be divided into three contributions, namely, correlation, non-hole-hopping relaxation, and hole-hopping relaxation. In the case of atomiclike localized levels, the deeper the level, the more the non-hole-hopping (static) relaxation dominates over the hole-hopping (dynamical) relaxation (DR). In the former relaxation, the initial hole remains in the same orbital and acts as a classical static charge, inducing the radial distortions of the surrounding electrons, i.e., monopole relaxation. The non-hole-relaxation energy shift is fairly independent of the angular momentum quantum number [22–27] of a hole created in the same atomic subshell. This is because the non-hole-hopping relaxation involves the radial distortions which are independent of the angular momentum quantum number of the hole. On the other hand, in the latter relaxation the hole fluctuates between different orbitals, in other words, the initial single-

TABLE I. X-ray emission transitions of xenon (in eV). Δ1= transition energies determined from single-hole BE's. *L*-shell BE's used were determined from expt. XES and XPS of final states (Ref. [6]); see text and Table II. Δ2=Δ1−expt. XES. Δ3=DHFΔSCF−expt. XES.

Line	Expt. XES	Δ1	DHFΔSCF[c]	Δ2	Δ3
$L_l(L_3M_1)$	3 636.9(3)	3 638.2	3 635.7	1.3	−1.2
$L\eta(L_2M_1)$	3 957.8(2)	3 957.5	3 956.0	−0.3	−1.8
$L\alpha_2(L_3M_4)$	4 097.42(5)	4 097.6	4 098.4	0.13	0.98
$L\alpha_1(L_3M_5)$	4 110.18(4)	4 110.2	4 111.7	0.02	1.52
$L\beta_1(L_2M_4)$	4 417.66(2)	4 416.9	4 418.7	−0.81	1.04
$L\beta_4(L_1M_2)$	4 450.36(2)	4 450.3	4 454.1	−0.06	3.74
$L\beta_3(L_1M_3)$	4 511.98(4)	4 511.8	4 516.3	−0.18	4.32
$L\beta_2(L_3N_5)$	4 718.86(8)	4 719.4	4 721.0	0.54	2.14
$L\gamma_1(L_2N_4)$	5 037.14(10)	5 036.7	5 039.3	−0.44	2.16
$L\gamma_3(L_1N_3)$	5 306.7(2)[a]	5 306.9	5 302.9	0.2	−3.8
$K\alpha_2(KL_2)$	29 458.44(9)[b]	29 458.4	29 459.0	0	0.56
$K\alpha_1(KL_3)$	29 778.97(5)[b]	29 778.7	29 779.3	−0.3	0.33
$K\beta_3(KM_2)$	33 563.42(12)[b]	33 563.4	33 561.2	0	−2.22
$K\beta_1(KM_3)$	33 624.45(12)[b]	33 624.9	33 623.4	0.5	−1.05

[a] Reference [2].
[b] Reference [8].
[c] Reference [21].

hole (lh) and the intermediate two-hole–one-particle ($2h$-$1p$) configuration correlate strongly, including nonspherical (angular) distortions of the surrounding charge densities. The dominant part of the hole hopping relaxation is the so-called dipole relaxation. The DR energy shift can be very large.

A large part of the relaxation of a localized hole in the atomic like system is due to non-hole-hopping relaxation and it can be described well by the DHFΔSCF method [22–27]. This is the main reason why the DHFΔSCF method often gives good agreement with experimental energy, although the DHFΔSCF method does not take into account the correlations and hole hopping relaxation. The difference between the correlations in the initial neutral ground state and final ionic state tends to be small (order of 1 eV), thus the major part of the aforementioned significant discrepancy between the experiment and DHFΔSCF energies cannot be attributed only to correlation energy shifts. The present experimental x-ray emission energy shows a larger deviation from the DHFΔSCF results (Table I, column 6) when the initial or (and) final hole is the orbital which satisfies $l<n-1$ (for $n=1$, 2, and 3) and $l<n-2$ (for $n=4$ and 5), where l is the angular momentum quantum number and n is the principal quantum number of the hole, namely L_1, M_1, $M_{2,3}$, and $N_{2,3}$. However, there is a smaller deviation when the hole does not satisfy the above relationship. This implies a possibility of relaxation which depends on the angular momentum quantum number, namely the (dynamical) hole-hopping relaxation. The large discrepancy observed in the present results must be mainly due to a DR energy shift which is totally neglected by the DHFΔSCF method.

B. Ionization energies

For an analysis of the relaxation and correlation energy shift of each atomic level, it is more instructive to consider the XPS hole energy rather than the XES emission energy. In Table II we list the hole energies determined by XPS, XANE, and XES. Using the accurately measured XPS BE's for the atomic levels of Xe up to a BE of 1148.7 eV ($3s$ level), we determine the L_1, $L_{2,3}$ BE's from the present XES data. The resulting BE's are in good agreement with earlier [1] XPS data.

A comparison of the experimental XPS BE's with the DHFΔSCF results shows an expected discrepancy from the above discussion on the DR shift. For the outermost orbital of the subshell, the deviation is small and positive. However, in the case of other orbitals, the deviation trend is larger and negative. This is because for the outermost orbitals of the subshell, the hole-hopping DR within the same subshell [e.g., $nl^{-1}\leftrightarrow n(l+1)^{-1}n(l+2)^{-1}\varepsilon(l+3)$ Coster-Kronig (CK), $nl^{-1}\leftrightarrow n(l+1)^{-2}\varepsilon(1+2)$ super-CK processes, including excitations to discrete states] does not occur, and hole-hopping DR which involves the different subshell is often very small. Thus the correlation energy shift will not be canceled out or reduced by the DR energy shift. The deviation between the XPS and DHFΔSCF BE is due mainly to the correlation energy shift neglected by the DHFΔSCF method. On the other hand, in the case of inner orbitals, the DR would give rise to a significant energy shift. The sum of the DR and correlation energy shift often reduces the BE and becomes the difference between the XPS and DHFΔSCF BE. To summarize, the deviation between the experimental and DHFΔSCF energies for the outermost shell is due mainly to the correlation energy shift and that for the inner shell is DR energy shift. in the present case, the dominant DR is due to super-Coster-Kronig processes e.g.,

$$2s^{-1}\leftrightarrow 2p^{-1}3d^{-1}\varepsilon f\ ,$$
$$3s^{-1}\leftrightarrow 3p^{-1}3d^{-1}\varepsilon f\ ,$$
$$3p^{-1}\leftrightarrow 3d^{-2}\varepsilon f, 4s^{-1}\leftrightarrow 4p^{-1}4d^{-1}\varepsilon f\ ,$$
$$4p^{-1}\leftrightarrow 4d^{-2}\varepsilon f\ ,$$
$$5s^{-1}\leftrightarrow 5p^{-2}\varepsilon d\ .$$

Here it should be noted that the continuum electron has the largest possible orbital angular momentum which often gives a larger $1h-2h$-$1p$ coupling matrix element than the one which has a smaller angular momentum.

One of the methods to calculate the DR energy shift is the Green's-function method. By describing the $1h-2h$-$1p$ configuration interaction (CI) in terms of the self-energy of a hole, one can then describe the energy positions and lifetime broadening of the spectrum in a consistent way. (Refer to [22–27] for details of method and numerical procedure.) In the present work we calculated the BE's of the $3s$, $3p$, and $5s$ levels of Xe by the extended random-phase-approximation with exchange (RPAE) Green's-function method. Comparison with experiment is in excellent agreement. We list also the ionization energies by Chen *et al.* [29], who calculated the DR energy shift. By adding their calculated DR energy shifts to the DHFΔSCF values, and also adding the estimated correlation energy shift (which would increase the BE by about 1 eV), the agreement with experiment is also good.

We should comment on the calculation scheme used by Chen *et al.* [29] for the DR shift. These authors used Fano's approach of CI of the $1h$ with the $2h$-$1p$ continuum; however, the equation they solved is the Dyson equation for the diagonal second-order self-energy. Their "self-energy" includes the following approximations. For the evaluations of the $1h-2h$-$1p$ coupling matrix elements, Chen *et al.* [29] used the initial single-hole relaxed orbitals for the occupied orbitals and the construction of the potential to generate the unoccupied (continuum) orbitals. This approach is based on the two-step model whereby one separates the primary photoionization and the secondary Auger emission process. This approach is justified when the relaxation of the initial hole is much shorter than the time scale of the Auger decay of the core hole. Since the initial state of the excitation is a neutral ground state and not the initial single-hole relaxed state, the use of neutral ground-state wave functions is a reasonable choice for the Green's-function method which is based on a one-step model description of the ionization processes. The interaction between the two holes created by an Auger or CK transition and the particle (Auger or

TABLE II. Binding energies of xenon single-hole levels (in eV). $\Delta 4 = \mathrm{XES} - \mathrm{DHF}\Delta\mathrm{SCF}$. $\Delta 5 = \mathrm{XPS} - \mathrm{DHF}\Delta\mathrm{SCF}$.

Level	Present work (XES)	XPS	XANE	DHFΔSCF[e]	Δ4	Δ5	Ohno	Chen *et al.*[i]
$K(1s)$	34 565.5(3)			34 566.8	−1.3			
$L_1(2s)$	5 452.2(2)	5453.2(4)[a]	5452.9(5)[d]	54 59.7	−7.5	−6.5	5452.8[f]	
$L_2(2p_{1/2})$	5 107.1(5)	5107.2(4)[a]	5107.0(5)[d]	5 107.8	−0.7	−0.6		
$L_3(2p_{3/2})$	4 786.8(5)	4787.3(4)[a]	4786.3(6)[d]	4 787.5	−0.7	−0.2		
$M_1(3s)$		1148.7(5)[b]		1 151.8		−3.1	1148.7[h]	1149.8
		1148.4[j]						
$M_2(3p_{1/2})$		1002.1(3)[b]		1 005.6		−3.5	1003.6[h]	1004.5
$M_3(3p_{3/2})$		940.6(2)[b]		943.4		−2.8	941.6[h]	941.5
$M_4(3d_{3/2})$		689.35(8)[b]		689.1		0.3		
$M_5(3d_{5/2})$		676.70(8)[b]		657.8		0.9		
$N_1(4s)$		213.32(3)[b]		222.7		−9.4	214.7[g]	213
$N_2(4p_{1/2})$				169.2				
$N_3(4p_{3/2})$		145.51(2)[b]		156.8		−11.3	146.3[g]	145.3
$N_4(4d_{3/2})$		69.48(1)[b]		68.5		1		
$N_5(4d_{5/2})$		67.50(1)[b]		66.5		1		
$O_1(5s)$		23.40(1)[b]		26.5		−3.1	23.3[h]	
$O_2(5p_{1/2})$		13.43(1)[b]		12.54		0.90		
$O_3(5p_{3/2})$		12.127[c]		11.23		0.90		

[a] Reference [1].
[b] Reference [6].
[c] Reference [28].
[d] Reference [5].
[e] Reference [21].
[f] Reference [2].
[g] References [22,23].
[h] Present work.
[i] Reference [29].
[j] Reference [34].

CK continuum electron) is treated within the RPAE in order to include the polarization due to the hole-particle pair excitations. The interaction becomes fairly important for low-energy hole-particle excitations but has been totally neglected in their scheme. In the extended RPAE Green's-function method the $1h$-$2h$-$1p$ coupling matrix element is renormalized by treating the $1h$-$1p$ interaction with the RPAE. In the extended RPAE method the screening and relaxation of the double hole in $2h$-$1p$ is treated within the framework of the DHFΔSCF scheme. However Chen *et al.* used the approximate double-ionization energies.

Although the Green's-function method and the approach of Chen *et al.* used different approximations, the calculated DR energy shifts are very similar. This is not surprising since the 1h-state solution of the Dyson equation lies in the energy region where the real part of the self-energy shows a smooth behavior, which is rather independent of the choice of wave functions (e.g., frozen core or relaxed), or potential [e.g., HF V^{N-2}, (Tamm-Dancoff approximation (TDA), or Hartree-Fock-Slater (HFS) V^{N-1}), etc. One thereby obtains similar results in spite of different approximations. However, in the case of the hole lifetime, the calculated lifetime is often very sensitive to a choice of approximations. It is very important to include correlations in the calculation scheme (see later).

The $4s$ and $4p$ levels of Xe and surrounding elements experience very strong dynamical relation and decay processes. Spectra that involve the $4p$ hole as the final hole in the emission transition show strong dynamical effects [2,9–11]. These spectra have been calculated by the extended RPAE Green's-function method and are in good agreement with the measured spectra [2,10,11,27].

C. Widths

In Table III are listed the corrected widths of the measured x-ray emission transitions in this work. The fitted diffraction line in the parallel position $(1,-1)$ was taken as the instrumental broadening distribution in the spectral region of interest. The diffraction line was Lorentzian with FWHM values ranging as cited above in Sec. II. The spectral-line profiles were Lorentzian or near Lorentzian. The measured L-emission linewidths were corrected by subtracting the instrumental FWHM from the fitted spectral-line FWHM.

The widths of the L levels were determined on the assumption that the width of the corrected emission lines is the linear sum of the initial and final hole states. Krause and Oliver [30] determined the K and L widths also from K XES and KLL AES spectra. In the process of the determination of the widths, they assumed that the spectral function of the final two-hole state is given simply by the convolution of that of each hole of the final state. This is valid only when the interaction between the two holes can be neglected, which is when the holes are delocalized. Certainly this is not true in the case of free atoms. The L-level widths listed in Table IV are the average values determined from the experimental L XES widths in Table III and their corresponding final state widths from Table IV. The broader Ll and $L\eta$ lines were

TABLE III. Expt. L XES widths of Xe (in eV).

Line	FWHM
$L_l(L_3M_1)$	13.36
$L\eta(L_2M_1)$	11.47
$L\alpha_2(L_3M_4)$	3.52
$L\alpha_1(L_3M_5)$	3.44
$L\beta_1(L_2M_4)$	3.41
$L\beta_4(L_1M_2)$	6.00
$L\beta_3(L_1M_3)$	7.43
$L\beta_2(L_3N_5)$	3.10
$L\gamma_1(L_2N_4)$	2.95
$L\gamma_3(L_1N_3)$	3.7

not included in this determination.

We list also in Table IV the widths calculated by other investigators. The calculation by one of the authors were performed by the extended RPAE Green's-function method. Using this method one can calculate also the line profile of the spectrum which can deviate considerably from a Lorentzian profile (e.g., $4p$ XPS spectrum of Xe) [22,23,27]. In contrast to the conventional method which calculates the widths using the golden rule, the Green's-function method takes into account the renormalization of the width by the pole strength and strong energy dependence of the imaginary part of the self-energy in the energy region of the pole to describe more accurately the decay width. This becomes essential when the spectral profile deviates very much from a Lorentzian profile. For some levels, we see a significant deviation between experiment and theory. We will discuss the origin of these discrepancies in the remaining portion of this section.

As demonstrated in a comparison with experiment for a wide range of atomic elements [31], the first extensive calculations of the decay widths by McGuire [32] were unsuccessful when the hole involves the strong dynamical decay process (often in the inner-shell levels where the DR is not negligible). Note the results for the L_1, M_1, $M_{2,3}$, N_1, and $N_{2,3}$ levels of Xe. Many-body effects in the CK decay and treatment of these effects by a many body theory such as the Green's-function method have been already emphasized in previous works [23–27]. A comprehensive discussion on the causes of the discrepancies that occurred in the calculations by McGuire [32] and Chen *et al.* [33] can be found in previous works on decay widths [23–26]. Here we comment briefly on the major causes of the discrepancies.

The Auger-decay transition matrix elements calculated by McGuire [32] have been used extensively by several authors for the calculations of the intra-atomic-Auger-transition in decay rates in atoms, solids and molecules. The results for $L_{2,3}$ $M_{4,5}$, and $N_{4,5}$ levels are often in reasonably good agreement with experiment in spite of several approximations made by McGuire [32] for the evaluation of the Auger decay rates. This is because the Auger energies are often large, and the interaction between the two holes and the escaping Auger electron is

TABLE IV. FWHM (eV) of xenon single-hole levels.

	Expt.		Theory			
Level	XES	XPS[a]	Krause and Oliver[b]	Ohno	McGuire[e]	Chen *et al.*[f]
$K(1s)$	11.4		11.4			11.43
$L_1(2s)$	3.0		3.64		4.08	3.524
$L_2(2p_{1/2})$	2.9		3.40		3.48	3.049
$L_3(2p_{3/2})$	2.9		3.13		2.68	2.823
$M_1(3s)$		8.0		7.24[c]	10.18	
		7.1[g]				11.64[g]
$M_2(3p_{1/2})$		3.2		3.11[c]	4.83	
$M_3(3p_{3/2})$		3.9		3.85[c]	5.48	
$M_4(3d_{3/2})$		0.5			0.68	
$M_5(3d_{5/2})$		0.5				
$N_1(4s)$		2.7		2.8[d]	5.49	
$N_2(4p_{1/2})$		smeared out		smeared out	2.56	
$N_3(4p_{3/2})$		1.0		0.5[d]	2.56	
$N_4(4d_{3/2})$		0.1			0.082	
$N_5(4d_{5/2})$		0.1			0.082	
$O_1(5s)$		0.05				
$O_2(5p_{1/2})$		<0.05				
$O_3(5p_{3/2})$		<0.05				

[a] Reference [1].
[b] Reference [30].
[c] Reference [24].
[d] References [22,23].
[e] Reference [32].
[f] Reference [33].
[g] Reference [34].

relatively small and not very important. Thus the auger decay rates are often insensitive to the choice of potentials used to generate the wave functions and the degree of approximations used to describe the correlations. Therefore the results by McGuire [32] and Chen *et al.* [33] usually give good agreement with experiment for the outermost hole levels of an arbitrary subshell, the decay of which is dominated by the Auger decay processes (e.g., $L_{2,3}$, $M_{4,5}$, and $N_{4,5}$ levels of Xe). However, in the case of CK decay, the decay processes involve the holes in the same atomic subshell. Then the CK decay energy is often small, and the interaction between the two holes and the CK electron is very important. The CK decay rates become very sensitive to a choice of potential and the approximations to describe such strong interactions. The calculations by McGuire [32] and Chen *et al.* [33] completely neglect such many-body effects. In contrast the Green's-function method includes these many-electron effects to some extent by a well-established perturbation expansion scheme. In general, therefore, the calculation of the normal Auger transition rates cannot be used as a critical test of the validity of the calculation scheme, whereas the calculation of the CK decay rates can serve as a useful criterion to test a scheme.

McGuire [32] and Chen *et al.* [33] used relaxed orbitals for their calculations. The use of relaxed orbitals is problematic. In order to use a relaxed orbital, one has to assume that the Auger decay starts when the system is almost or fully relaxed. The static monopole relaxation energy shift of the core levels for Xe is appreciably larger than the decay width (the shift is about 190, 50, and 19 eV for *K*, *L*, and *M* shells, respectively). In this case one may justify the use of relaxed orbitals of the initial hole state. However, for the *N* shell, the static relaxation shift is about 6 eV, and the DR shift can be as much as 12 eV. In the case of the 4*p* hole the super-CK decay time is so rapid that the quasiparticle picture breaks down completely. In this case the decay and relaxation are not separable, and a consistent treatment of the width and energy shift is necessary to calculate the relaxation and decay consistently [22,23,27]. Using the relaxed orbitals may sometimes lead to a better agreement with experiment. However, this does not fully justify the approach itself, particularly when important correlation effects are neglected. These comments also apply when discussing relativistic effects. Without a proper treatment of the correlations, one is not able to discuss the relativistic effects even when one obtains a better agreement with experiment by including the relativistic effects. Very recently Mäntykentta *et al.* [34] have calculated the 3*s*-decay width of atomic Xe by using the Dirac-Fock wave functions (employing the same scheme by Chen *et al.* [33]) Their result of 11.64 eV is more than 50% larger than the experimental width [34] of 7.1 eV. Their result is quite close to the calculated value by McGuire [32], who used a similar scheme. On the other hand, the Green's-function calculations of the M_1 widths of the elements Kr to Xe give excellent agreement with experiment. In Table IV is the Green's-function method calculated M_1 width for xenon of 7.24 eV. This shows that the relativistic effects are not significant and that the many-body effects such as polarization due to hole-particle pair excitations play a much more important role in the determination of the Coster-Kronig decay.

IV. CONCLUDING REMARKS

In the present work we measured the *L* x-ray emission spectra of Xe and analyzed the widths and energies by comparing with other available experimental and theoretical data. The discrepancies between theory and experiment are interpreted in terms of the dynamical relaxation and decay. This discrepancy can be mended by using a many-body approach such as the Green's-function method by which one can treat such strong correlations in a consistent way. In the present work the BE's of 3*s*, 3*p*, and 5*s* levels of Xe are calculated by the Green's-function method, offering good agreement with experiment. The present interpretation of the relaxation energy is based upon the perturbation scheme within the Hartree-Fock method. The non-hole-hopping and hole-hopping relaxation terms appear also in the *g*-Hartree method [35]. In this method, the *g* value is obtained so that all relaxation and correlation terms become zero. The variation of the *g* value in different atomic shell excitations reflects the variation of different kinds of relaxation involved in the excitation process [36].

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