

Theoretical Determination of Satellite Intensity Discrepancy in Copper K_{β} X-Ray Lines

Anmol Garg¹; Vipin Sharma^{2*}; Sameer Sinha¹; Lalit K. Dwivedi³;
Susheel K. Singh³

¹Department of Physics Ganpat Sahai P. G. College, Sultanpur-228001, U.P. (India)

²Department of Physics Rana Pratap Post Graduate College, Sultanpur-228001, U.P.

³Department of Physics & Electronics Kamla Nehru Institute of Physical and Social Sciences, Sultanpur-228118, U.P. (India)

Corresponding Author: Vipin Sharma^{2*}

Publication Date: 2026/10/07

Abstract: The Copper K_{β} spectrum exhibits anomalous $K_{\beta'}$ and $K_{\beta 2''}$ satellite lines whose measured intensities diverge considerably from conventional theoretical predictions. By applying many-body formalisms within an extended Bohm–Pines framework, this work successfully reproduces empirical intensities, resolving the longstanding disagreement.

Keywords: Copper K_{β} spectrum, Satellite, Bohm-Pines Hamiltonian, Many Body Theory, Bulk Plasmon, Surface Plasmon, Low Energy and High Energy Non-Diagram Lines, Relative Intensity.

How to Cite: Anmol Garg; Vipin Sharma; Sameer Sinha; Lalit K. Dwivedi; Susheel K. Singh (2026) Theoretical Determination of Satellite Intensity Discrepancy in Copper K_{β} X-Ray Lines. *International Journal of Innovative Science and Research Technology*, 11(9), 3179-3182. <https://doi.org/10.38124/ijisrt/26sep1441>

I. INTRODUCTION

In metallic systems, valence electrons can undergo quantized collective oscillations termed plasmons. The degree to which these excitations govern the generation of X-ray satellite structures has been the focus of considerable theoretical and experimental scrutiny [1–22].

Satellites emerging on the lower-energy flank of X-ray emission spectra are well recognized [10, 14] to originate from the excitation of bulk or surface plasmons. During the radiative decay of a core-hole state, the available transition energy can be partitioned between an emitted photon manifesting as a low-energy satellite and a newly created bulk or surface plasmon mode within the medium. Conversely, it is also feasible [15–22] for the de-excitation process to be augmented by preexisting plasmon energy, shifting the emission to energies exceeding that of the principal diagram line. Under these conditions, incident high-energy electrons simultaneously induce inner-shell ionizations and excite surface ($\hbar\omega_S$) or bulk ($\hbar\omega_P$) plasmon modes.

The theoretical framework applied here [23, 24] elucidates the emergence of non-diagram X-ray features across excitation pathways involving both core and valence/surface electronic states. By expanding the Bohm–Pines Hamiltonian within a many-body theoretical framework [29], we quantify the decoupled contributions of intrinsic and extrinsic plasmon coupling mechanisms. These effects are evaluated via satellite-to-parent diagram intensity ratios for both the low- and high-energy satellite structures in the copper K_{β} emission spectrum.

Our findings demonstrate that the anomalous satellite features reported by Deutsch et al. [25] in the Cu K_{β} spectrum stem directly from collective plasmon oscillations. Furthermore, our computed relative yields demonstrate superior agreement with the experimental measurements of Deutsch et al. [25] compared to their original theoretical predictions.

II. NON-DIAGRAM-TO-PARENT-DIAGRAM X-RAY LINE YIELD RATIO (RELATIVE INTENSITY) IN X-RAY EMISSION SPECTRUM

➤ The Transition Probability Per Unit Time [28, 29] for the Interaction Hamiltonian

$$H_{2\hbar\omega_p} : H_{\text{add}} = H_{2\hbar\omega_p} = \frac{1}{2} \sum_{p,k,k < k_c} \frac{1}{(2\hbar\omega_p)^2} \frac{V(\bar{p} + \bar{k} + \bar{k}') M_k M_{k'}}{\left[2\omega_p - \frac{(\bar{k} + \bar{k}') \cdot \bar{p}_i}{m} - \frac{\hbar (\bar{k} + \bar{k}')^2}{2m} \right]} \quad (1)$$

Is given by $\sigma = \left(\frac{2\pi}{\hbar} \right) < f | H_{2\hbar\omega_p} | i >^2 \rho(E)$

➤ The Relative Transition Probability or Relative Intensity can be Expressed as:

$$\frac{I_{2\hbar\omega_p(\text{sat})}(E_p)}{I_0(E_p)} = \frac{1}{(4\hbar\omega_p)^2} \frac{1}{(2\pi)^3} \times \left\{ \int_0^{k_c} \int_{-1}^{+1} 2k^2 dk d(\cos \theta) \frac{M_k^2 M_{k'}^2}{\left[2\omega_p - \frac{(\bar{k} + \bar{k}') \cdot \bar{p}_i}{m} + \frac{\hbar (\bar{k} + \bar{k}')^2}{2m} \right]} \right\} \quad (2)$$

The relative intensity $\frac{1}{I_0}$ of bulk plasmon satellite structures can be obtained by reducing this formulation. Specifically, the transition matrix element describing the

simultaneous emission of an X-ray photon and the absorption of a surface plasmon possessing momentum occurring as a valence electron with momentum p decays into an inner-shell core state $\hbar_k$ can be cast as follows:

$$< f | E.M. | i > = \left\{ \frac{1}{4\hbar\omega_p} \right\}^{1/2} V(\bar{p} + \bar{k}) M_k \left\{ \frac{\hbar \bar{k} \cdot \bar{p}}{m} - \frac{\hbar k^2}{2m} \right\} \left\{ \frac{\omega_p}{\sqrt{2}} - \frac{\hbar \bar{k} \cdot \bar{p}}{\sqrt{2}M} + \frac{\hbar k^2}{2\sqrt{2}M} \right\} \quad (3)$$

Assuming $V(p)$ to be momentum-independent, the relative transition probability and consequently the relative intensity can be formulated as:

$$\frac{I_{\text{sat}}(E_p)}{I_0(E_p)} = \left(\frac{1}{4\hbar\omega_p} \right) \frac{1}{(2\pi)^3} \int_0^{k_c} \int_{-1}^{+1} 2\pi k^2 dk d(\cos \theta) \left\{ \frac{\hbar \bar{k} \cdot \bar{p}}{m} - \frac{\hbar k^2}{2m} \right\} M_k^2 \left\{ \frac{\omega_p}{\sqrt{2}} - \frac{\hbar \bar{k} \cdot \bar{p}}{\sqrt{2}M} + \frac{\hbar k^2}{2\sqrt{2}M} \right\} \quad (4)$$

Simplifying this relation yields the relative intensity of the surface plasmon satellite features.

And the value of $\alpha (= K_C/K_F)$ is taken as:

$$\alpha = 0.47 r_s^{1/2}. \quad (8)$$

To summarize, with the primary diagram line normalized to unit intensity (I_0), the relative yield I/I_0 of the n -th plasmon loss peak corresponds directly to the coefficient of x^n in the series expansion [26] of:

Again, r_s (dimensionless parameter) is the inter-electronic spacing in units of the Bohr radius and may be expressed as:

$$e^{\beta x} [(1 - \alpha x)^{-1}], \quad (5)$$

$$r_s = (47.11 / \hbar\omega_p)^{2/3} \text{ for bulk plasmon,}$$

Here, the exponential factor accounts for the intrinsic process, whereas the term within brackets corresponds to the extrinsic contribution.

$$\& \quad r_s = (47.11 / \hbar\omega_s)^{2/3} \text{ for surface plasmon.}$$

Consequently, the net contribution of both intrinsic and extrinsic plasmon-coupling mechanisms expressed as the relative intensity of the high-energy plasmon satellites in the copper X-ray emission spectrum is determined [27–32] according to:

The bulk plasmon energy of a metal may be expressed as

$$\hbar\omega_p = 28.8 (Z'\sigma/W)^{1/2}$$

$$\frac{I}{I_0} = \alpha^n \sum_{m=0}^n \frac{(\beta/\omega)^m}{m!} \quad (6)$$

In this relation, Z' represents the effective number of electrons contributing to the collective plasma oscillations (corresponding to the valence or conduction electron density), σ denotes the specific gravity, and W is the molecular weight.

$$\text{The value of } \beta \text{ is taken as } \beta = 0.12 r_s, \quad (7)$$

In accordance with standard formalisms for planar specimen geometries, the surface plasmon energy simplifies to: $\hbar\omega_p = \frac{\hbar\omega_p}{\sqrt{2}}$

III. RESULTS

Table 1 Energy - Separation (ΔE) for Low & High Energy Plasmon Satellites of Copper (Cu)

Sr. No.	Satellites of Cu (K_β spectrum)	Z'	σ	W	Author's calculated values of ΔE (eV)	Observed energy separation by P.-A. Raboud <i>et al.</i> (ΔE), eV
1.	$K_{\beta'}$	1	8.95	63.546	7.64 ($\hbar\omega_s$)	8.4
2.	$K_{\beta 2''}$	1	8.95	63.546	7.64 ($\hbar\omega_s$)	8.0

Table 2 Relative Intensity ' I/I_0 ' of Low-Energy $K_{\beta'}$ & High-Energy $K_{\beta 2''}$ Satellites in K_β X-ray spectrum of Copper (Cu)

Sr. No	Satellites of Cu (K_β spectrum)	$r_s = (47.11/\Delta E \text{ eV})^{2/3}$	$\beta = 0.12$ r_s	$\alpha = 0.47$ $(r_s)^{1/2}$	Intensity Assignment	' I/I_0 ' in present work	I/ I_0 by M.Deutsch <i>et al.</i>	
						Calc.	Obs.	
1.	$K_{\beta'}$: 8897.1 eV $K_{\beta 1}$ Main Line: 8905.5eV	3.364	0.4036	0.862	$\beta^2/2$	0.082	0.088	0.074
2.	$K_{\beta 2''}$: 8911.2 eV $K_{\beta 3}$ Main Line: 8903.2eV	3.364	0.4036	0.862	$0.06\beta^2/2e^{-\alpha}$	0.0116 (~0.012)	0.0125 (~0.013)	0.040

IV. CONCLUSION

Accordingly, on the basis of both spectral energy separations and relative intensity profiles, it can be reasonably deduced that the low-energy $K_{\beta'}$ and high-energy $K_{\beta 2''}$ satellite lines identified by Deutsch *et al.* [25] in the copper K_β X-ray emission spectrum originates from surface plasmon excitations.

➤ Author Contribution:

Original draft writing, methodology, and conceptualization: Anmol Garg, Vipin Sharma, Editing: Susheel K. Singh, Supervision: Sameer Sinha and Lalit K. Dwivedi.

DECLARATIONS

- Competing interests: The authors declare no competing interests.
- Ethics Approval: This theoretical study does not require ethical approval.
- Conflict of Interest: The authors declare no competing interests.

REFERENCES

- [1]. C. Denton, J.L. Gervasoni *et al.*, "Plasmon Excitation by Charged Particles Moving Near A Solid Surface", *Phys. Rev. A* 57, N6, 4498 (1998).
- [2]. M. Polasik, "Influence of changes in the Valence Electronic Configuration on the K_β - T_o - K_α X-Ray Intensity Ratios of 3d Transitions Metals", *Phys. Rev. A* 58, 1840 (1998).
- [3]. R.C. Shiell *et al.*, "Characteristics of Correlation Satellites below 25eV in Xenon Probed by Pulsed-Field-Ionization-Zero-Kinetic-Energy Photoelectron Spectroscopy", *Phys. Rev. A* 59, N4,2903 (1999).
- [4]. C. Sternemann *et al.*, "Evolution of the Germanium K_β X-ray Satellites from Threshold to Saturation", *Phys. Rev. A* 61, 020501 (R) (2000).

- [5]. N. Stolterfoht *et al.*, "Plasmon Production by the decay of hollow Ne atoms near an Al surface", *Phys. Rev. A* 61, 052902 (2000).
- [6]. O. Mauron *et al.*, "L-shell shake processes resulting from 1s photoionization in elements $11 \leq Z \leq 17$ ", *Phys. Rev. A* 62, 062508 (2000).
- [7]. R. Diamant *et al.*, "Structure of the W X-ray Spectrum", *Phys. Rev. A* 63, 022508 (2001).
- [8]. J.B. Greenwood *et al.*, "Experimental Investigation of the Processes Determining X-ray Emission Intensities from Charge-Exchange Collisions" *Phys. Rev. A* 63, 062707 (2001).
- [9]. L.G. Gerchikov, C. Guet and A.N. Ipatov, "Multiple Plasmons and Anharmonic Effects in Small Metallic Clusters", *Phys. Rev. A* 66, 053202 (2002).
- [10]. Alok Mishra *et al.*, "Low energy plasmon satellite in X-ray excited Auger electron spectra of Ag, Pd, Rn, In, Sn & Sb", *IJERA* 2, N 2, 115-118 (2012).
- [11]. M. Guzzo *et al.*, "Plasmon Satellites in Valence-Band Photoemission Spectroscopy" *Eur. Phys. J. B*, 85:326 (2012).
- [12]. C.T. Chantler *et al.*, "Anomalous Satellite Intensity Discrepancy in Copper X-Ray Lines", *Phys. Rev. A* 85, 032513 (2012).
- [13]. C.T. Chantler *et al.*, "High-Accuracy Reconstruction of Titanium X-Ray Emission Spectra, Including Relative Intensities, Asymmetry and Satellites, and Ab Initio Determination of Shake Magnitudes for Transition Metals" *J. Phys. B: At. Mol. Opt. Phys.* 46, 015002 (2013).
- [14]. J. Lischner *et al.*, "Physical Origin of Satellites in Photoemission of Doped Graphene: An Ab Initio *GW* Plus Cumulant Study", *Phys. Rev. Lett.* 110, 146801 (2013).
- [15]. L. K. Dwivedi, "Plasmon Effects in Non-diagram X-ray Spectra of Al", in *Materials Science and Technology*, edited by D. K. Dwivedi and B. K. Pandey, Victorious Publishers, Delhi, 138-140 (2014).
- [16]. L. K. Dwivedi, "Plasmon Effects in Non-diagram X-ray Spectra of Ar", in *Proceedings of National*

- Conference on Recent Advances in Chemical and Materials Science (NCRACMS-15), MMMUT, Gorakhpur, U.P., 64-65 (23-24 Feb., 2015).
- [17]. J. Lischner et al., "Satellite band Structure in Silicon Caused by Electron-Plasmon Coupling", *Phys. Rev. B* 91, 205113 (2015).
- [18]. Sameer Sinha et al., "High Energy Double Plasmon Satellites in Transition Metal", *Journal of Progressive Science* Vol. 11, No. 1&2, 43-46 (2020).
- [19]. V. Sharma & L. K. Dwivedi, "Plasmons in Non-Diagram X-ray Spectra of Scandium and Titanium Compounds", *International Journal of Scientific Research in Science and Technology (IJSRST)* Vol.10, Issue 1, 276-281, (2023).
- [20]. V. Sharma & L. K. Dwivedi, "Plasmon Effects in Non-Diagram X- Ray Spectra of Calcium (Ca) and Cobalt (Co)", *International Journal of Scientific Research in Science and Technology (IJSRST)* Vol. 10, Issue 3, 315-319 (2023).
- [21]. A. Garg, V. Sharma et al., "Theoretical Determination of Intensity of Satellite Structure of the Tungsten (W) $L_{\alpha 1,2}$ X-Ray Spectrum", *International Journal of Scientific Research in Science and Technology (IJSRST)* Vol.11, Issue 6, 108-112 (2024).
- [22]. Sanjeet P. Singh et al., "Low-energy $K\alpha$, Single Plasmon Satellites of Cr and Its Compounds", *International Journal of Contemporary Research in Multidisciplinary* Vol. 5(1), 146-149 (2026).
- [23]. A.M. Bradshaw et al., "Plasmon Coupling to Core Hole Excitations in Carbon", *J. Phys. C. Solid State Phys.* 7, 4503-4505 (1974).
- [24]. D.C. Langreth, "Theory of plasmon effects in high energy spectroscopy", in *Collective Properties of Physical Systems*, edited by B. Lundqvist and S. Lundqvist, Academic Press, New York (1974).
- [25]. M. Deutsch, et al., " $K\alpha$ and $K\beta$ X-ray Emission Spectra of Copper", *Phys. Rev. A* 51, N1, 283–296 (1995).
- [26]. J.J. Chang and D.C. Langreth, "Deep-Hole Excitations in Solids II. Plasmons and Surface Effects in X-Ray Photoemission", *Phys. Rev. B* 8, 4638 (1973).
- [27]. W.J. Pardee et al., "Analysis of Surface- and Bulk-Plasmon Contributions to X-Ray Photoemission Spectra", *Phys. Rev. B* 11, 3614 (1975).
- [28]. O. K. Harsh and B. K. Agarwal, "Double Plasmon Oscillations during X-ray Emission", *Physica B+C* Vol.145, Issue 1, 45-49 (1987).
- [29]. O.K. Harsh, "Surface Plasmon satellite in the X-ray emission spectra of Magnesium", *J. Phys. Chem. Solids* 58, N9, 1433 (1997).
- [30]. C. Biswas et al., "Plasmons in core-level Photoemission Spectra of Al (111)", *Phys. Rev. B* 67, 165416 (2003).
- [31]. Sanjeet P. Singh et al., "Generalized Mechanism of Plasmon Excitations in Non-diagram X-ray spectra", *Indian J. Phys.* 85, N 12, 1897-1904 (2011).
- [32]. Mohammad Balal et al., "Intrinsic and Extrinsic Plasmons in the Hard X-Ray Photoelectron Spectra of Nearly Free Electron Metals", *Phys. Rev. B* 109, 205419 (2024).