SOFT X-RAY EMISSION SPECTRUM OF METALS*†

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When a metal is excited through prior bombardment by x rays or electrons, removing one of the valence-band electrons, an electron in the conduction band can drop into the valence hole with the emission of a soft x ray. The intensity of x-ray emission as a function of the x-ray frequency gives a measure of the width of the conduction band of the metal and of the conduction-electron density of states.[1] However, the determination of these properties is compounded by electron-electron interactions which modify the spectrum and give it a tail which obscures the conduction-band width. In addition, interactions give rise to collective behavior such as plasma production. This behavior is reflected in the spectrum[2,3] as a satellite emission band which appears at lower energy since the plasmon excitation leaves less energy available for the emission process. Previous attempts[4-6] to incorporate such interaction effects into the theory have led to results which are considerably stronger than the experiments indicate.[7,2] We have applied the apparatus of diagrammatic many-body theory to this problem and have found that the earlier treatments have overlooked important interference terms. When these terms are retained the agreement with experiment is excellent.

The x-ray emission intensity is proportional to the electron transition rate

$$w=\frac{1}{l}\sum_{i,f}|\langle\Psi_f|\sum_{k=1}^{N}\hat{n}\cdot\vec{p}_k|\Psi_i\rangle|^2\delta(\omega+E_f-E_i), \qquad (1)$$

where one sums over all possible final states and averages over initial states, l being the number of initial states. The transition matrix elements for coupling with the electromagnetic field are taken between the exact wave functions of the many-body system. Here $\hat{n}$ is a unit vector in the direction of the field. E_i and E_f are the exact energies of the initial and final states. The exact states are not known, but can be approximated using the apparatus of many-body theory with selected summations of terms in the perturbation series.

It is convenient to rewrite Eq. (1) as the real part of an integral over a correlation function

$$w=\frac{1}{\pi l}\sum_i \mathrm{Re}\int_0^\infty dt\, e^{i\omega t}\langle\Psi_i|\mathcal{O}^+(t)\mathcal{O}(0)|\Psi_i\rangle, \qquad (2)$$

where

$$\mathcal{O}(t)=e^{iHt}\hat{n}\cdot\vec{p}\,e^{-iHt}. \qquad (3)$$

The correlation function,

$$\langle\Psi_i|\mathcal{O}^+(t)\mathcal{O}(0)|\Psi_i\rangle, \qquad (4)$$

can be expressed in terms of Feynman graphs in the usual way.[8] Typical graphs which occur in the present case are shown in Fig. 1. The initial configuration of the system contains a hole in one of the core levels. Such a hole is represented in the figure by a downward directed double line. The other directed lines correspond to conduction-band states and can be directed upward or downward depending on whether the line represents a particle in a level above the Fermi surface or a hole within the Fermi sea, respectively. The wavy line ending in an X depicts the interaction with the radiation field, and the line of bubbles indicates the dy-

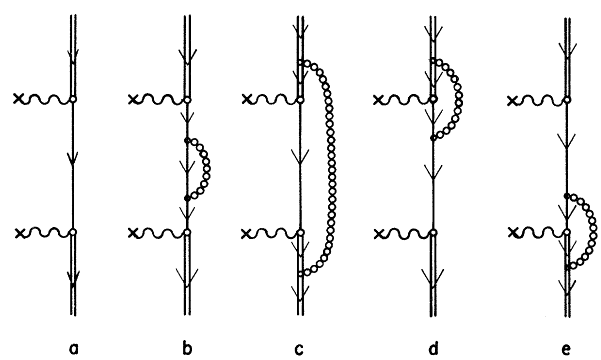

FIG. 1. Typical graphs which contribute to soft x-ray emission.

namic effective interaction between electrons[8]:

$$\mathcal{V}(\vec{k},\omega)=v(\vec{k})/\epsilon(\vec{k},\omega), \tag{5}$$

where $v(\vec{k})$ is the unscreened Coulomb interaction and $\epsilon(\vec{k},\omega)$ is the frequency and wave-number dielectric constant of the electron gas in the Lindhard approximation.

Figure 1(a) is of zero order in the electron-electron interaction and represents the emission as given by the Sommerfield model. The next graph, shown in Fig. 1(b), allows for interaction between electrons in the conduction band. Such terms were considered earlier by Landsberg,[4] although he calculated the interaction using a static screened potential which did not allow for plasmon production. These corrections give a finite width to the conduction-electron states and hence lead to a low-energy tail on the emission spectrum. However, if one uses the accepted Bohm-Pines screening length in the potential, then the tailing is much too strong. Indeed, the emission band melts into a broad weak continuum. Landsberg was able to circumvent this difficulty and obtain rough agreement with experiment by using a screening length of about half the Bohm-Pines value. The third contribution, Fig. 1(c), tends to increase the tailing still further, roughly doubling it. This term arises from a scattering or excitation of a conduction-band electron by the hole in the core state. The hole acts as a positively charged impurity in the metal which excites the conduction electrons virtually. When the x ray is emitted it has a lowered energy since some energy is left behind to make the virtual excitations real. Terms equivalent to these were included by Pirenne and Longe[6] in a static approximation. They calculated the effect of Auger processes which leave secondary conduction electrons in excited states as the potential in which they move changes suddenly as the x ray is emitted and the core impurity disappears. They also included the Landsberg process in their calculations, but were forced to use a still smaller screening length and to renormalize the spectrum in order to get agreement with experiment.

The main difficulty with these previous calculations appears to be the neglect of Figs. 1(d) and 1(e). These additional graphs are interference terms. They arise from a cross product between a matrix element for core excitation of the conduction band and for conduction-electron interaction. These new terms are of the same order of magnitude as (b) and (c) but of opposite sign. As a result, the net tailing and plasmon effect is sharply reduced and much more in accord with experiment.[1,9,3]

Detailed calculations of these effects were carried out for the $L_{\mathrm{II,III}}$ emission spectrum of Na. In this case the valence hole is one of the $2p$ states, and the conduction electrons fill a spherical Fermi sea. The conduction-electron wave functions are taken as plane waves orthogonalized to the core states. However, the orthogonalizing terms are retained only in matrix elements including a bound-state wave function. Thus we neglect complications associated with keeping the conduction-band wave functions orthogonalized, and momentum is conserved in conduction-electron collisions. Any errors introduced by these approximations appear to be minor. The $2p$ state functions and the orthogonalizing parts of the conduction states are constructed from hydrogenic-type wave functions using Slater's[10] rules for the variational parameters. The resulting wave functions are in excellent agreement with wave functions constructed by the Wigner-Seitz procedure.[11] They have strongly $3s$ character close to the ion core, but remain essentially plane waves over 90% of the lattice cell. The energy of the bound state is taken from data of Skinner[1] as 27.3 eV below the bottom of the conduction band.

Results for the tailing and the plasmon satellite are plotted in Fig. 2. The plasmon satellite reflects the main emission band except that it is shifted to lower frequencies due to the energy retained by the plasmon excitation

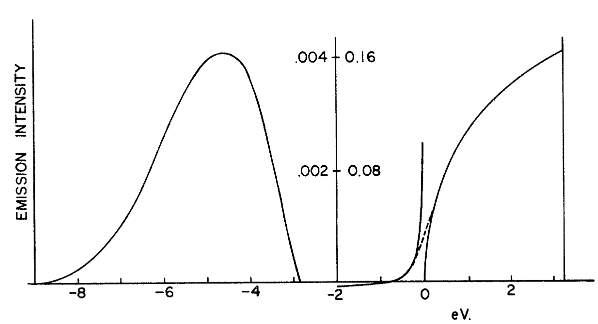

FIG. 2. Emission intensity in arbitrary units as a function of energy measured in electron volts from the bottom of the zero-order (Sommerfeld model) band edge. Note the difference in scale between the main band with its interaction tail, shown on the right of the scale, and the plasmon satellite band shown on the left.

in the metal. It is broader and the peak is shifted to a lower relative energy than the main band due to the wave-number dependence of the plasmon energy. The intensity of the satellite is about 2% of that of the main band, in agreement with Rooke's observations.[3] The tailing extends about 1 eV below the main emission band in accord with Skinner's observations. It arises from the incoherent single-electron excitation of the metal. It should fit smoothly onto the main emission band and fall off smoothly to zero at lower frequencies. Calculations of the effect of interactions on the main emission band and of how the tail merges with it are still in progress. In these regions, higher order graphs play an important role in canceling out divergences in the perturbation series. For consistency they also should be considered at lower frequencies where the tail becomes vanishingly small. The strong cancellation between the terms we have considered makes higher order terms non-negligible by comparison. Indeed, the present calculations give a slightly negative tail for energies more than 1 eV below the main band in contradiction to the positive definiteness of Eq. (1). However, for this region the tailing is already so weak compared to the main band that the corrections to these results are only of interest for determining the intensity background for the plasmon satellite band.

A more detailed report on these effects is being prepared.

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TEST OF CHARGE-CONJUGATION INVARIANCE IN $\bar{p}$-p ANNIHILATIONS AT REST*

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The violation of *CP* invariance has been observed by Christenson et al.[1] in K^0 decay. Several authors have suggested that this result may be the consequence of the violation of *C* invariance in the strong interactions.[2-4] We report here a search for such a violation in the annihilations of antiprotons at rest in hydrogen. The best tests heretofore of *C* conservation in the strong interaction are tests of time-reversal invariance. This is equivalent if *CTP* invariance is assumed, since parity conservation in the strong interaction is demonstrated with great precision. No violation of *T* invariance has been reported. The experiments on p-p triple scattering[5] show that the *T*-nonconserving amplitude should be no more than 3% of the *T*-conserving amplitude. Detailed balance experiments[6] find that *T*-nonconserving amplitudes should be no more than 2 to 3% of the *T*-conserving amplitudes.