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Threshold Behavior of the Soft-X-Ray Spectra in Metals*

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The behavior of soft-x-ray emission and absorption spectra near the Fermi-limit threshold is considered. Realistic parameters have been calculated for the Nozières–de Dominicis solution to a simplified model for the soft-x-ray process which is valid near the threshold. It is shown that for simple metals these parameters are only weakly dependent upon the particular metal and that it is the *symmetry* of the x-ray transition matrix element which is of essential importance in determining the threshold behavior. It is found that $L_{2,3}$ spectra tend to be enhanced near the threshold, whereas K spectra tend to fall smoothly to zero. This result is in accord with the observed emission spectra of the light elements, and appears to explain the "anomalous" K spectrum of Li as well as the high-energy peak in the $L_{2,3}$ spectrum of Na.

I. INTRODUCTION

SOFT-X-RAY absorption and emission spectra of metals have been extensively studied for many years. In terms of a one-electron model the absorption spectra yield direct information about the unoccupied energy levels of the conduction band, whereas emission spectra give information about the occupied portion of the band. However, it has long been recognized[1–7] that electron interactions play an important role in modifying the low-energy side of the emission spectrum, giving rise to a tail which obscures the width of the conduction band and a collective resonance (plasmon production) which is reflected in the spectrum as a satellite band. The high-energy end of the emission spectrum (and low-energy end of the absorption spectrum) of metals was expected to display a sharp threshold corresponding to the edge of the Fermi distribution of conduction electrons. In practice the sharpness of the threshold is modified by thermal broadening and the effect of the finite width of the deep x-ray level. However, some spectra display structure near the threshold which cannot be explained by the usual broadening mechanisms or by structure in the density-of-states curves. A prime example is the emission spectrum of Li,[8–11] which displays a premature peak about 0.65 eV below the high-energy threshold (see Fig. 1). Even the Na emission spectrum[1,12] (Fig. 2), whose sharp high-energy edge is well accounted for by a one-electron theory, exhibits a definite enhancement near threshold which cannot be accounted for by the Na density-of-states curve which follows quite closely the ideal $E^{1/2}$ energy dependence throughout the occupied portion of the conduction band.

The K x-ray emission of Li results from the radiative transition of a conduction electron to a vacant $1S$ level, whereas the $L_{2,3}$ x-ray emission of Na results from a transition to a vacant $2P$ level. The premature peak in the Li emission spectrum was first noticed by O'Bryan and Skinner[8] in 1934 and confirmed in subsequent measurements by Bedo and Tomboulian,[9] Catterall and Trotter,[10] and Crisp and Williams.[11] This anomaly has attracted considerable theoretical attention. The most accurate band calculations[13] for Li confirm that there is no contact of the Fermi surface with the Brillouin zone and that the density-of-states curve is increasing near the Fermi surface. Goodings[14] ascribed the observed shape of the Li spectrum to a change in

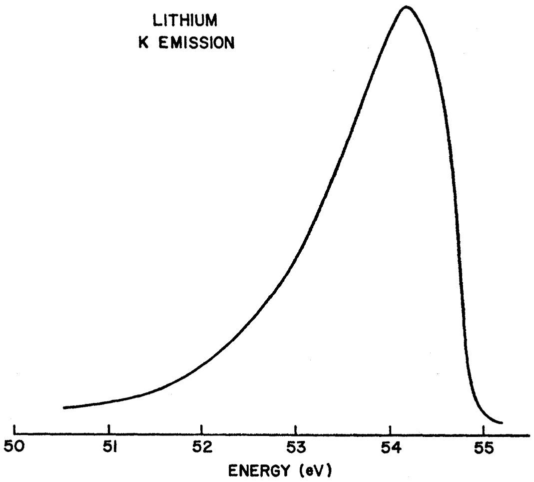

FIG. 1. K emission spectrum of Li (after Ref. 11).

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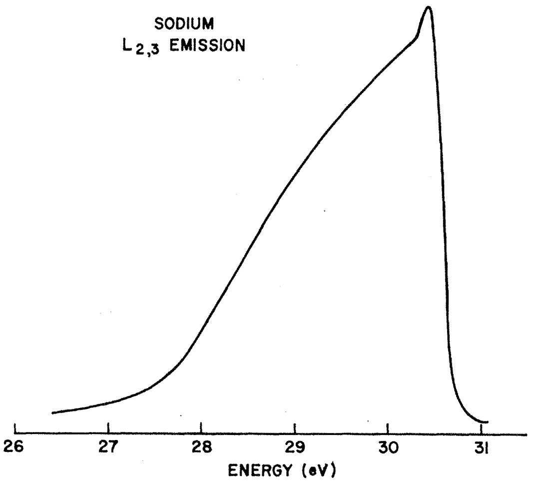

FIG. 2. $L_{2,3}$ emission spectrum of Na (after Ref. 12).

density of states in the presence of the $1S$ hole. By expanding the perturbed wave functions in terms of Wannier wave functions and using a Koster-Slater-type localized approximation he arrived at a "weighted" density-of-states function. He showed that in the presence of a bound state the wave functions at the perturbed atom acquire more localized character at the expense of the band wave functions, resulting in a falloff in the weighted density-of-states function near the Fermi energy. This qualitatively explains the intensity falloff of the emission spectrum near the Fermi energy. Shuey[15] has considered both the band structure of Li and the scattering of the conduction electrons from the screened Coulomb field of the $1S$ hole in the first Born approximation. He suggested that the premature peak in the x-ray intensity is due to the distortion of the Block wave functions by the $1S$ hole. The resulting spectrum is considerably enhanced over the zero-order spectrum and the concavity of the spectrum near the Fermi threshold is reversed. The most quantitative theory of the Li spectrum proposed so far is that of Allotey,[16] who simultaneously considered the Na spectrum. By constructing a Hartree-type potential for the Li ion with $1S$ hole and computing the scattering wave functions for the electrons inside the Wigner-Seitz sphere, he found that the shape of the Li spectrum can be qualitatively explained if a p-wave scattering resonance exists in the band near the Fermi level. He concluded from his calculations that a p-wave scattering resonance does exist. Since conduction electrons with p symmetry are not involved in the $L_{2,3}$ emission of Na, no anomalies in the Na spectrum were found. While these one-electron theories give possible explanations for the Li premature peak, no one-electron theory has been proposed to explain the threshold peak in Na. A possible many-particle explanation was implicit in the work of Pirenne and Longe,[3] who considered the effect of double electron transitions which leave the system in an excited state following the emission of the x ray. While they were primarily interested in the low-energy tail of the emission spectrum, their calculation also reveals a divergence at the threshold. However, this singular behavior is obscured in their final result by the introduction of a deep level width which is too large. More recently Mahan[17] and Mizuno and Ishikawa[18] rediscovered this divergence and extrapolated from a third-order treatment of the x-ray absorption problem to predict that the absorption spectrum should diverge at the absorption threshold as an inverse power law of $\omega-\omega_0$, where $\omega-\omega_0$ is the difference between the x-ray absorption energy and the threshold energy. This behavior was then put on a firmer basis and corrected by Nozières and de Dominicis[19] (ND) who found an exact solution to a simplified[18,20] model of the soft-x-ray emission and absorption spectra in metals which is valid near the Fermi-level threshold. The more exact treatment of the problem by ND shows that the x-ray transition rate near threshold behaves as $\epsilon^{-\alpha}$, where $\epsilon=\omega-\omega_0$ for absorption and $\epsilon=\omega_0-\omega$ for emission, and α is a function of the phase shifts which describe scattering of the conduction electrons by the hole in the x-ray level. α may be positive or negative, leading, respectively, to an infinite or zero x-ray intensity at threshold. Thus this theory raises the possibility of explaining the threshold behavior of Li and Na within the same framework. We have examined the phase shifts and transition matrix elements for these metals and found that the theory does indeed give results in qualitative accord with the observed spectra.

The ND model consists of a gas of electrons spread over a continuum of conduction states and a single deep-lying x-ray level. Interactions between the conduction electrons are neglected; however, the electrons are scattered by the localized ionic potential when the deep state is empty. The Hamiltonian is

$$H=\sum_{\mathbf{k}} \epsilon_{\mathbf{k}} a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}}+E_B b^{\dagger} b+\sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}'} b b^{\dagger}, \qquad (1)$$

where $\epsilon_{\mathbf{k}}$ is the conduction electron energy, E_B is the energy of the deep level, $a_{\mathbf{k}}^{\dagger}$ and $b^{\dagger}$ are creation operators for a conduction electron and for the deep-state electron, respectively, and $V_{\mathbf{k},\mathbf{k}'}$ is the matrix element for scattering of an electron from state $\mathbf{k}'$ to $\mathbf{k}$ by the deep-state hole. X-ray emission or absorption is induced by the term

$$H_x=\sum_{\mathbf{k}} W_{\mathbf{k}} a_{\mathbf{k}}^{\dagger} b e^{-i\omega t}+\text{c.c.}, \qquad (2)$$

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which causes an electron to make a transition from a conduction state to the bound state or vice versa. Since the operators b, $b^\dagger$ appear quadratically in Eq. (1), the model is equivalent to a "one-body" problem with an effective potential

$$V=\sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'}a_{\mathbf{k}}^\dagger a_{\mathbf{k}'}-E_B\,, \tag{3}$$

which is switched off or on at the moment of the x-ray transition. It is this feature, that the scattering potential V is time-dependent, that makes the model nontrivial to solve. The ND solution gives the transient response of the conduction electrons to the abrupt change in potential. They find that the transition rate is proportional to

$$R(\epsilon)=\sum_{lm}|W_{lm}|^2\left(\frac{\xi_0}{\epsilon}\right)^{\alpha_l}, \tag{4}$$

where ξ_0 is a cutoff energy, the W_{lm} are the coefficients of the expansion of the x-ray matrix element in spherical harmonics, and the α_l are given in terms of the phase shifts δ_l for scattering of the conduction electrons (at the Fermi energy) by the deep-hole state,

$$\alpha_l=2\frac{\delta_l}{\pi}-2\sum_l(2l+1)\left(\frac{\delta_l}{\pi}\right)^2. \tag{5}$$

If one or more of the α_l in Eq. (4) is positive and the associated W_{lm} is nonzero, then the transition rate should be infinite at threshold. However, if all of the contributing α_l are negative, then the transition rate should go to zero as $\epsilon\rightarrow 0$ and there should be no sharp threshold. In Sec. II physical arguments are given which lead to the conclusion that for simple metals the *signs* of the α_l are independent of the particular metal. This conclusion is borne out by explicit evaluation of the phase shifts for Li and Na. Thus, knowledge of the W_{lm} is of crucial importance in determining which l values contribute to the sum in Eq. (4), and hence in determining whether the spectrum diverges to infinity or goes to zero at the threshold energy. Whether or not a given W_{lm} vanishes is determined by the symmetry of the dipole matrix element. The symmetry of the K and $L_{2,3}$ transition matrix elements is discussed in Sec. III and the W_{lm} are determined. We conclude from the symmetry arguments that $L_{2,3}$ emission spectra should diverge to infinity at the high-energy threshold while K emission spectra should go continuously to zero. This result is in accord with the observed emission spectra of several of the light metals and gives an alternative explanation for the K emission spectrum of Li as well as an explanation for the high-energy peak in the $L_{2,3}$ emission spectrum of Na.

II. PHASE-SHIFT ANALYSIS

It is known from quantum-mechanical scattering theory that the phase shifts δ_l become quite small for values of $l\gtrsim ka$, where a is a measure of the range of the scattering potential and k is related to the particle energy by $\epsilon_k=\hbar^2k^2/2m$. For an electron at the Fermi energy of a metal, moving in a screened Coulomb potential with screening length q_s^{-1}, the condition on the relevant l values is approximately $l\lesssim k_0/q_s$, where k_0 is the Fermi momentum. q_s is given by $q_s^2=(12/\pi)^{2/3}/r_sa_0^2$, where a_0 is the Bohr radius, r_s is a measure of the electron density, $r_s=r_0/a_0$, and r_0 is the radius of a sphere equal in volume to the volume per electron. Since $k_0=(9\pi/4)^{1/3}/a_0r_s$, the condition on the l values in terms of r_s is $l\lesssim(9\pi/4)^{2/3}/3r_s^{1/2}=1.23/r_s^{1/2}$. For typical metals $2<r_s<6$. Thus $0.5<l_{\max}<0.9$, and s-wave scattering should predominate. The Friedel sum rule

$$\sum_{l=0}^{\infty}(2l+1)\delta_l=\tfrac{1}{2}\pi \tag{6}$$

imposes restrictions on the phase shifts for scattering of electrons in a metal. If δ_0 is, indeed, the dominant phase shift, then the Friedel sum rule requires $\delta_0\simeq\frac{1}{2}\pi$ and $\delta_l\simeq 0$ $(l\neq 0)$ which leads to the conclusion [from Eq. (5)]

$$\alpha_0>0\,,\quad \alpha_l<0\ (l\neq 0)\,. \tag{7}$$

This conclusion will now be verified by explicit evaluation of the phase shifts for Li ($r_s=3.28$) and Na ($r_s=3.96$).

The generalization of the ND equation for the $l=0$ phase shift to arbitrary l values is

$$\tan\delta_l(\epsilon_{\mathbf{k}})=\frac{\Omega\pi}{2l+1}V_l(k,k)\rho(\epsilon_{\mathbf{k}})\bigg/\left(1-\frac{4\pi}{2l+1}\frac{\Omega}{(2\pi)^3}\times\int_0^\infty dk'k'^2\frac{P}{\epsilon_{\mathbf{k}'}-\epsilon_{\mathbf{k}}}V_l(k',k')\right), \tag{8}$$

where $\rho(\epsilon_{\mathbf{k}})$ is the density-of-states function and

$$V_l(k,k')=\frac{2l+1}{2}\int_{-1}^{1}d\mu P_l(\mu)V_{\mathbf{kk}'}\,. \tag{9}$$

The $P_l(\mu)$ are the Legendre polynomials and μ is the cosine of the angle between $\mathbf{k}$ and $\mathbf{k}'$. Equation (8) was derived for a potential for which each Legendre component is separable;

$$V_l(k,k')=V_lU_l(k)U_l(k')\,, \tag{10}$$

where $U_l(k)$ is a cutoff function more or less centered on the Fermi surface and such that $U(k_0)=1$. For the present calculation it is desirable to choose a model potential which incorporates parameters characteristic of the particular materials under investigation. We retain Eq. (8), but we replace $V_l(k,k')$ by a more

TABLE I. Phase shifts δ_l and exponents α_l for Li and Na.

	Li		Na			
	($g=0.596$)		$m=0$ ($g=0.638$)		$m=\pm1$ ($g=0.549$)	
l	δ_l	α_l	δ_l	α_l	δ_l	α_l
0	9.54×10^{-1}	0.409	9.21×10^{-1}	0.398	1.04	0.433
1	1.49×10^{-1}	−0.104	1.63×10^{-1}	−0.085	1.33×10^{-1}	−0.148
2	2.48×10^{-2}	−0.183	2.44×10^{-2}	−0.173	1.94×10^{-2}	−0.220
3	4.95×10^{-3}	−0.196	4.37×10^{-3}	−0.186	3.46×10^{-3}	−0.230
4	1.07×10^{-3}	−0.198	8.43×10^{-4}	−0.188	6.70×10^{-4}	−0.232

realistic, though unseparable, function. The interaction of conduction electrons with the bound state hole is given by

$$V_{\mathbf{k}\mathbf{k}'}=\int d^3x\int d^3x' u_{\mathbf{k}}^*(\mathbf{x})u^{B*}(\mathbf{x}')\times V(\mathbf{x},\mathbf{x}')u^B(\mathbf{x}')u_{\mathbf{k}'}(\mathbf{x}). \quad (11)$$

If the $u_{\mathbf{k}}$ are approximated by plane waves[21]

$$u_{\mathbf{k}}(\mathbf{x})=\Omega^{-1/2}e^{i\mathbf{k}\cdot\mathbf{x}},$$

then

$$V_{\mathbf{k}\mathbf{k}'}=\int d^3x'|u^B(\mathbf{x}')|^2e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{x}'}\frac{1}{\Omega}\int d^3x e^{-(\mathbf{k}-\mathbf{k}')\cdot\mathbf{x}}V(\mathbf{x})$$

$$\equiv\frac{1}{\Omega}f(\mathbf{k}-\mathbf{k}')\tilde{V}(\mathbf{k}-\mathbf{k}'), \quad (12)$$

where $\tilde{V}(\mathbf{k}-\mathbf{k}')$ is the Fourier transform of $V(\mathbf{x})$. We take $V(\mathbf{x})$ to be the usual screened Coulomb potential whose Fourier transform is

$$\tilde{V}(\mathbf{k}-\mathbf{k}')=4\pi e^2/(|\mathbf{k}-\mathbf{k}'|^2+q_s^2). \quad (13)$$

The form factor $f(\mathbf{k}-\mathbf{k}')$ assumes the task of the $U_l(k)$ in suppressing the contribution to the interaction from high momentum components. This is a reflection of the fact that the charge density of the deep-state vacancy is not punctual, but has a finite extension in space. The phase shifts calculated using this potential are too large, more than exhausting the Friedel sum rule. To force agreement with this condition an adjustable strength parameter g was introduced and varied until the first five phase shifts ($\delta_4\simeq0.001\ \delta_0$) calculated from Eq. (8), using the potential $gV_l(k,k)$ satisfied the Friedel sum rule. The introduction of this parameter had little effect on the *relative* magnitudes of the phase shifts. The resulting phase shifts δ_l and exponents α_l are given in Table I. Since this work was carried out we have learned that Mahan[22] has independently calculated a set of phase shifts using a Fredholm-type method due to Noyes and finds δ_l's which are in essential agreement with those of Table I.

III. SYMMETRY OF THE MATRIX ELEMENTS

The dipole matrix element is given by

$$W(\mathbf{k})=\langle u_{\mathbf{k}}|\hat{n}\cdot\mathbf{p}|u_{nlm}{}^B\rangle, \quad (14)$$

where $u_{\mathbf{k}}$ is the conduction-electron wave function and $u_{nlm}{}^B$ is the bound-state wave function[23] with atomic quantum numbers nlm. For K emission $u_{nlm}{}^B$ is an s state, $u_{100}{}^B$. For $L_{2,3}$ emission $u_{nlm}{}^B$ is a p state and has the three components $u_{210}{}^B$ and $u_{21\pm1}{}^B$. The intensity in the latter case is obtained by averaging over the transitions with different m. The conduction-electron wave functions are taken to be plane waves orthogonalized to the core states of the excited ion. In the K emission of Li the orthogonalizing term which is subtracted from the plane wave has S symmetry. Hence its contribution to the dipole matrix element is zero, and the conduction-electron wave function appearing in the matrix element is effectively a plane wave. In Na the contributions to the matrix element from the orthogonalizing terms of P symmetry vanish; however, those with S symmetry could be important. The relevant core wave functions were constructed using Slater's rules.[24] For Li K emission the resulting matrix element is of the form

$$W(\mathbf{k})=W_{10}(k)Y_{10}(\hat{k}), \quad (15)$$

where Y_{lm} is the usual spherical harmonic, and the unit vector $\hat{k}$ is measured relative to the polarization vector $\hat{n}$ as the z axis. For Na the matrix element for a state of given m has the form[5]

$$W^{(m)}(\mathbf{k})=A\delta_{m0}Y_{00}(\hat{k})+B(k)Y_{10}(\hat{k})Y_{1m}(\hat{k}). \quad (16)$$

Combining spherical harmonics, the components can be written as

$$W^{(0)}(\mathbf{k})=W_{00}{}^{(0)}(k)Y_{00}(\hat{k})+W_{20}{}^{(0)}(k)Y_{20}(\hat{k}),$$
$$W^{(\pm1)}(\mathbf{k})=W_{2,\pm1}{}^{(\pm1)}(k)Y_{2,\pm1}(\hat{k}). \quad (17)$$

We need not concern ourselves with the explicit k dependence of the matrix elements. They are smoothly varying functions of k and act only as multiplicative factors in the transition rate. It is the *symmetry* of the matrix elements which is of essential importance here. Following ND we write

$$W_{lm}(k)=W_{lm}U_l(k), \quad (18)$$

where $U_l(k)$ is the same cutoff function as used in Eq. (10). Now we can substitute into Eq. (4) to obtain the energy dependence of the transition rate near threshold.

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[21] It is shown in Ref. 5 that this is a good approximation for this matrix element.

[22] G. D. Mahan (private communication).

[23] Here we neglect the small spin-orbit interaction which raises the degeneracy of the $2P_{3/2}$ and $2P_{1/2}$ states and gives rise to a slight splitting between L_2 and L_3 spectra. To include that effect one must use bound-state wave functions of the form $\psi(n,l,j,m_j)$. In the present context, however, where we average over initial states of different m, it makes no difference whether we use the $u(nlm)$ or the $\psi(n,l,j,m_j)$ as our basis.

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For the K emission of Li,

$$R(\epsilon)=|W_{10}|^2(\xi_0/\epsilon)^{\alpha_1}. \tag{19}$$

For the $L_{2,3}$ emission of Na,

$$\begin{aligned} R^{(0)}(\epsilon)&=|W_{00}{}^{(0)}|^2(\xi_0/\epsilon)^{\alpha_0}+|W_{20}{}^{(0)}|^2(\xi_0/\epsilon)^{\alpha_2},\\ R^{(\pm1)}(\epsilon)&=|W_{2,\pm1}{}^{(\pm1)}|^2(\xi_0/\epsilon)^{\alpha_2}. \end{aligned} \tag{20}$$

Since Eq. (7) holds for both Li and Na, we see from Eqs. (19) and (20) that the Li spectrum should go smoothly to zero as $\epsilon\rightarrow 0$, and thus possesses no sharp threshold though the slope is infinite at the edge, whereas the Na spectrum should diverge to infinity at threshold and then drop discontinuously to zero.

IV. SUMMARY AND DISCUSSION

The spectra calculated above are found with a model which includes the scattering of the conduction electrons by the transient core potential, but which omits several other physical processes which can strongly affect the spectra of real metals. An estimate of their importance can be obtained from the work of Bose, Glick, and Longe (BGL).[25] BGL included many-body effects in the calculation of the x-ray emission spectrum of Na by using a renormalized perturbation theory and going to first order in the effective interaction between particles. They found that the first-order correction to the radiation vertex gives a logarithmic singularity at threshold, but the singularity is made finite by the inclusion of the deep-hole lifetime (Auger broadening). The more accurate power-law behavior of the ND solution would also be made finite if the model were generalized to include a lifetime for the inner state. Nevertheless, the spectrum found in Ref. 25 retains a finite peak near threshold as evidence of the singular interaction between conduction electrons and the localized hole. Since the ND solution diverges as a power law rather than logarithmically, one might expect that even with lifetime effects included the spectrum should exhibit a similar or even somewhat greater enhancement near threshold.

For K emission a perturbation treatment of the BGL type is not possible even when lifetime effects are included. The perturbation treatment leads to a logarithmically divergent behavior at threshold, whereas the ND solution shows that the spectrum must go smoothly to zero at threshold. We are presently investigating what effect the inclusion of the hole lifetime and conduction-electron interactions would have on the present results, and how rapidly the K spectrum should drop to zero. In any case, the $L_{2,3}$ and K spectra should differ markedly near threshold.

As noted previously, the $L_{2,3}$ emission spectrum of Na exhibits a rather sharp high-energy threshold as well as a definite enhancement near threshold. On the other hand, the K emission spectrum of Li does not exhibit any enhancement and the threshold falloff is not as sharp. Thus, the theory seems to be in accord with the observed emission spectra. Extrapolating the results to other light metals, we note that Be has one electron more than Li (making its electron configuration $1S^2\,2S^2$) and would be an insulator except for the existence of band overlap. For this reason it is a more complicated metal to analyze than Li. However, the symmetry of the x-ray matrix element is the same as that for Li and the ND model therefore predicts a threshold behavior for its K emission spectrum similar to that of Li. Similarly, the $L_{2,3}$ emission matrix elements for Mg and Al, which have, respectively, one and two more electrons than Na, have the same symmetry as the Na matrix elements. The theory, therefore, indicates a sharply enhanced spectrum at the threshold such as is observed in these elements. The fact that the spectra of these two metals exhibit considerable structure has been interpreted in terms of the density of states for the overlapping energy bands of conduction electrons.[26] Additional insight is given by the work of Catterall and Trotter,[27] who studied $L_{2,3}$ emission from liquid Al. They found that the spectrum retains a peak at threshold though other structure attributed to the periodicity of the lattice disappears on melting. The similarity between their spectrum and the spectrum of Na metal is remarkable, and suggests that the mechanism discussed in this paper is also active in the case of Al.

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[26] D. H. Tomboulian, in *Handbuch der Physik*, edited by S. Flügge (Springer-Verlag, Berlin, 1957), Vol. 30, pp. 246–304.

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