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THEORY OF MULTI-ELECTRON RECOIL EFFECTS ON X-RAY LINESHAPES OF
METALS*

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Although the possible importance of many-electron effects in the x-ray spectra of metals was emphasized by Friedel as early as 1952 [1], very little is known even today at a quantitative level about the role of either the electron-hole interaction or electron-electron interactions in shaping x-ray spectra.

Current interest in these effects centers on a change in self-consistent field model of final-state electron-hole interactions formulated by Nozieres and de Dominicis in 1969. In solving their model in an asymptotic limit, Nozieres and de Dominicis found singular enhancements of the absorption and emission spectra at the Fermi threshold [2].

We have gone beyond the asymptotic theory and have explored the "exact" lineshapes obtained by solution of the change in self-consistent field model [3-12]. These "exact" lineshapes depend on the detailed form of the final-state interaction and, in many cases, exhibit interesting qualitative features absent from the asymptotic theory. We have calculated the "exact" lineshapes for $N=5, 10, 20, 40$, and 80 s-waves or p-waves and have found that the lineshapes for infinite N can be easily extrapolated from the finite- N spectra [3].

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One of the most interesting results illustrates how absorption and emission spectra evolve from the free-electron limit to the exciton limit as the electron-hole interaction strength, as characterized by the Fermi energy phase shift δ_0 , increases (Fig. 1).

The recoil spectra of p-waves [6,7] also exhibit interesting structure (Fig. 2) when the condition for a p-wave resonance is met.

We have also obtained results for s-wave recoil (x-ray photoemission) [5], for satellite emission [8], for "forbidden" absorption and emission spectra [9], for photoemission near surfaces [10], and for Auger spectra [11]. Most recently we have explored the role of exchange in shaping absorption and emission spectra [12]. Interesting modifications of lineshapes occur as a result of exchange transitions corresponding to excitation of a core p-electron to a conduction p-orbital, with a simultaneous dipole transition between an s and a p conduction orbital.

Fig. 2. Recoil profile for p-waves subjected to a square-well final-state interaction, after Ref. [7].

Fig. 1. Emission ($E < 0$) and absorption ($E > 0$) spectra for a free electron metal experiencing a square-well final-state interaction of increasing strength, after Ref. [4]. Solid lines: theory; broken lines: screened exciton approximation; dotted lines: free electron approximation; dash-dot lines: asymptotic theory.

We conclude that, even within the change of self-consistent field approximation, x-ray spectra can be considerably richer in many-electron phenomena than once suspected. With the finite number of electron method [3], these spectra can be evaluated for realistic electron-hole interactions in free electron metals. Our preliminary results [10] indicate that metals with band structure can also be treated this way. However, theories of final-state interactions in metals will have to await significant theoretical progress in two areas: (i) the reliable determination of the screened potential of a core hole in a metal (which remains a subject of widespread disagreement among theorists) and (ii) realistic evaluation of the effects of electron-electron interactions.

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