

Lawrence Berkeley National Laboratory

Recent Work

Title

ELECTRONIC BAND STRUCTURE AND PHOTEMISSION: A REVIEW AND PROJECTION

Permalink

<https://escholarship.org/uc/item/22h3512x>

Author

Falicov, L.M.

Publication Date

1987-09-01



Lawrence Berkeley Laboratory

UNIVERSITY OF CALIFORNIA

Materials & Chemical Sciences Division

Invited paper presented at the 14th International
Conference on X-ray and Inner Shell Processes,
Paris, France, September 14-18, 1987, and to be
published in Journal de Physique

Electronic Band Structure and Photoemission: A Review and Projection

L.M. Falicov

September 1987

For Reference

Not to be taken from this room



LBL-23976
c.1

DISCLAIMER

This document was prepared as an account of work sponsored by the United States Government. While this document is believed to contain correct information, neither the United States Government nor any agency thereof, nor the Regents of the University of California, nor any of their employees, makes any warranty, express or implied, or assumes any legal responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by its trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof, or the Regents of the University of California. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof or the Regents of the University of California.

Invited paper presented at the 14th International Conference on X-Ray and Inner Shell Processes, Paris, France, Sept. 14-18, 1987. To be published in Journal de Physique.

ELECTRONIC BAND STRUCTURE AND
PHOTOEMISSION: A REVIEW AND PROJECTION

L. M. Falicov

Materials and Chemical Sciences Division
Lawrence Berkeley Laboratory
University of California
Berkeley, California 94720 U.S.A.
and
NORDITA
Blegdamsvej 17, DK-2100
Copenhagen Ø, Denmark

September 1987

*This work was supported in part by the Director, Office of Energy Research, Office of Basic Energy Sciences, Materials Sciences Division of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

Résumé. - On présente ici une revue brève des calculs des structures électroniques des solides, vis à vis l'interprétation des résultats de photoémission. Ces calculs sont de trois classes:

(i) calculs de la structure cristalline électronique des bandes, dont les électrons sont considérés comme particules indépendentes;

(ii) calculs des modifications introduites dans la structure électronique par la surface du solide;

(iii) calculs des propriétés des systèmes électroniques à N-corps, et des modifications produites dans le solide, pendant le procès de photoémission, par la corrélation dynamique des électrons.

Abstract. - A brief review of electronic-structure calculations in solids, as a means of interpreting photoemission spectra, is presented. The calculations are, in general, of three types:

(i) ordinary one-electron-like band structures, which apply to bulk solids and are the basis of all other calculations;

(ii) surface modified calculations, which take into account, self-consistently if at all possible, the presence of a vacuum-solid interface and of the electronic modifications caused thereby;

(iii) many-body calculations, which go beyond average-field approximations and consider dynamic rearrangement effects caused by electron-electron correlations during the photoemission process.

INTRODUCTION

In 1987 it is very generally accepted [1] that photoemission, in particular angle-resolved photoemission, is one of the most important tools for understanding the electronic structure of solids, surfaces, interfaces, adsorbates, overlayers, small particles, etc. i.e. a large variety of condensed-matter systems. The available tunable and polarizable light sources, as well as the angle-resolved and polarization-sensitive electron detectors have fulfilled all expectations of general usefulness and precision vested on them in the 1960's and 1970's, when they were first being developed. It is fair to say that, because of the photoemission technique, we have now a much better and deeper understanding of the electronic structure of condensed matter than we had before the technique was generally implemented.

The experiments have provided an enormous wealth of information. They have confirmed, in general, the postulates of the foundations of the Electronic Theory of Condensed Matter. Thus -- based on the fundamental postulates of Quantum Mechanics and the understanding of the interactions and correlations among electrons, and between electrons and nuclei -- a level of calculational sophistication has been reached where first-principles predictions of electronic and structural properties appear now possible [2]. This process of understanding is very symbiotic in character: experiments can very seldom be interpreted without the aid of theoretical calculations, whereas the suitability and accuracy of the calculations are always monitored, confirmed or denied, and constantly reassessed based on ever more accurate and sophisticated experiments.

The understanding of the electron photoemission process in solids is firmly based on four chapters of the Quantum Theory of Matter: (1) the Electronic Band Structure Theory of Crystals; (2) Surface Physics; (3)

Many-Body Quantum Theory; and (4) the Theory of Interaction of Radiation and Matter. Said in simpler words it is necessary to know (1) how electrons move in solids under the influence of periodic potentials; (2) how that motion is modified by the presence of a solid-vacuum interface; (3) how the electrons interact with one another, with lattice vibrations and with other collective modes both in the bulk and close to the surface; and (4) how the interaction between these highly correlated electrons with the electromagnetic radiation field results in their leaving the solid with well defined momentum, energy, polarization, and intensity. Given the complexity of the problem, comprehensive, total calculations of the whole photoemission process are, at this point, out of the question. It is nonetheless surprising -- and indeed highly gratifying -- to see how much can be calculated, how relevant those calculations are, and how sophisticated and detailed have become the experiments, which measure quantities considered only theoretically accessible a few years ago.

BAND-STRUCTURE CALCULATIONS

Given the basic understanding of the photoemission process, which goes back to Einstein [3], and the fundamental conservation laws of energy, k -vector and angular momentum, the zeroth-order approximation in the interpretation of the data is to assume that, throughout the process, the electrons are independent particles that satisfy Fermi-Dirac statistics. In the initial state they move in the solid under the influence of a constant, self-consistent, perfectly periodic crystal potential. Their stationary state of motion is defined by their k -vectors -- restricted to the lattice Brillouin Zone -- their spin polarization σ_i , and the one-particle energies $\epsilon_i(k, \sigma_i)$. Similarly, after photoemission, the emitted electron is characterized by its momentum $\hbar\vec{K}$, its spin polarization σ_f , and its energy

$$\epsilon_f(\vec{K}, \sigma_f) = \hbar^2 K^2 / 2m + \epsilon_V, \quad (1)$$

where ϵ_V is the one-electron vacuum level. Conservation of energy and k -vector yields

$$\epsilon_f(\vec{K}, \sigma_f) - \epsilon_i(\vec{k}, \sigma_i) - \hbar\omega = 0, \quad (2)$$

$$\vec{K}_{\parallel} = \vec{k}_{\parallel} + \vec{G}_{\parallel}, \quad (3)$$

$$\hbar^2 K_{\perp}^2 / 2m = [\epsilon_f(\vec{K}, \sigma_f) - \epsilon_V] - \hbar^2 (\vec{k}_{\parallel} + \vec{G}_{\parallel})^2 / 2m, \quad (4)$$

and, in the absence of spin-dependent scattering,

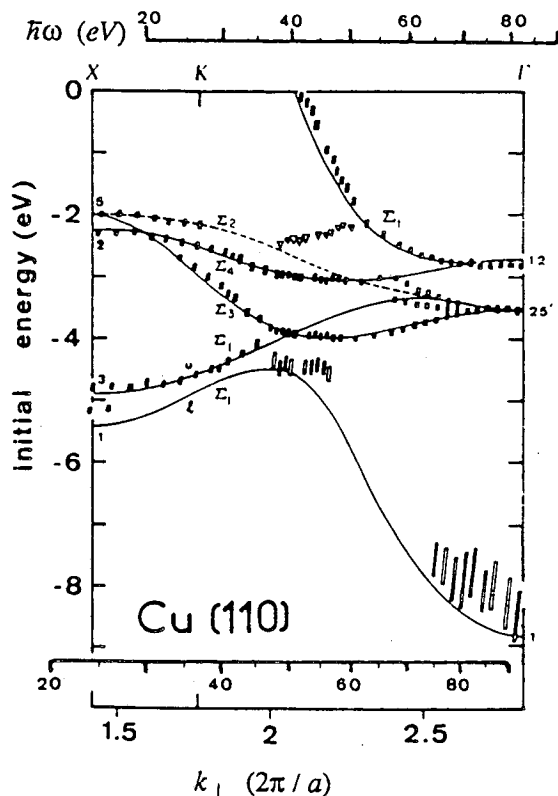
$$\sigma_f = \sigma_i. \quad (5)$$

In the equations above the subscripts \perp and \parallel indicate components perpendicular and parallel to the surface, respectively, and \vec{G} is one of the reciprocal lattice vectors.

It can be seen from (1)-(5) that, if ϵ_V and $\epsilon_i(\vec{k}, \sigma_i)$ are known, then, for each frequency ω , the kinetic energy, $\hbar^2 K^2 / 2m$, the direction of propagation (K_{\parallel}, K_{\perp}) -- within a reciprocal lattice vector -- and spin polarization σ_f of the photoemitted electron are uniquely determined. The inverse problem [4], the determination of $\epsilon_i(\vec{k}, \sigma_i)$ from measured energy, angle and polarization of the photoelectron is somewhat ambiguous because the component k_{\perp} of the initial k -vector does not appear in the equations above. This difficulty can be ameliorated in many instances by means of specific situations or by "bootstrapping" [4]. But, even if the inverse problem could not be completely solved, comparison between *calculated* one-electron energy curves $\epsilon_i(k, \sigma_i)$ and *measured* angle-resolved, photoelectron peaks can be made, and physical conclusions obtained from such comparisons.

The art of calculating the one-electron spectrum of perfect, crystalline solids has, by 1987, reached a very high level of sophistication [2, 5-7]. These calculations are based on very sound principles and, even though they are numerically intensive and laborious, they are very accurate and reliable. Discrepancies between various researches are either disappearing or, for all practical purposes, non-existing. It is therefore not surprising that in a large number of cases -- with few exceptions to be discussed below -- the comparison

Figure 1.
Experimentally determined valence-band structure for copper, for normal emission, along the $\Gamma - K - X$ line of the Brillouin zone [line perpendicular to the (110) surface]. The full curves correspond to the band structure calculated by Burdick [8]. The measured points are from the work of Thiry *et al.* [9]. The height of the rectangles gives the experimental uncertainty.



between existing band-structure calculations and detailed angle-resolved photoemission data is indeed very good [9,10]. An example of such excellent agreement is presented in Figure 1.

SURFACE CALCULATIONS

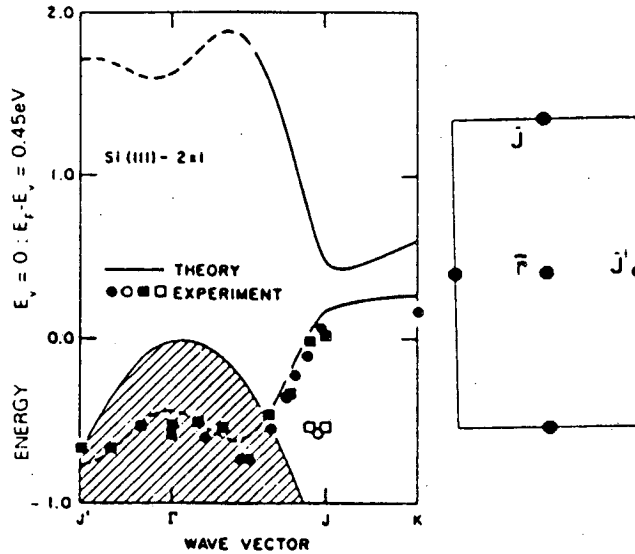
One of the attractive features of photoemission experiments is their surface sensitivity. The electrons emitted in the process are attenuated in the solid, mostly by energy losses caused by plasmon creation [11]. For electron energies of the order of 100 eV, the emitted electron originates, essentially, within a few -- typically 3 -- Ångstroms of the surface. For energies at least one order of magnitude larger or smaller, the attenuation length increases to about 20 Å. It is therefore possible, by tuning the frequency of the incoming radiation, to "tune" the region under examination "from surface to bulk". Even for attenuation lengths of the order of 20 Å the photoemitted electrons are strongly influenced by the surface. Therefore electronic "surface states" have a paramount influence on the photoelectric spectra. Surface states are one-electron orbitals which are localized in one dimension to the vicinity of the surface, while maintaining their itinerant character in the two directions parallel to it. Because they are essentially two-dimensional, they do not have a dependence on k_{\perp} and are easily identifiable experimentally [10]. Surface-state spectra are susceptible to special resonances [12].

The calculation of surface states, because of the removal of periodicity in one direction, is different but only slightly more complicated than that of bulk Bloch states. Comparison between theory and experiment for these surface states is also excellent. One example is given in Figure 2. It can be seen there that angle-resolved photoemission allows, by means of a successful comparison with a well defined and fully calculated structure, to accept a specific model of *surface reconstruction* and thereby decide between competing proposals and various theories.

The influence of the surface becomes paramount in cases where (a) there is a major surface reconstruction; (b) there are chemisorbed or physisorbed species on the surface; (c) there is segregation to the surface of one component of a multicomponent system; (d) there are -- naturally or artificially -- deposited overlayers [16] of a different material; and (e) there are strong magnetic effects at the surface [17].

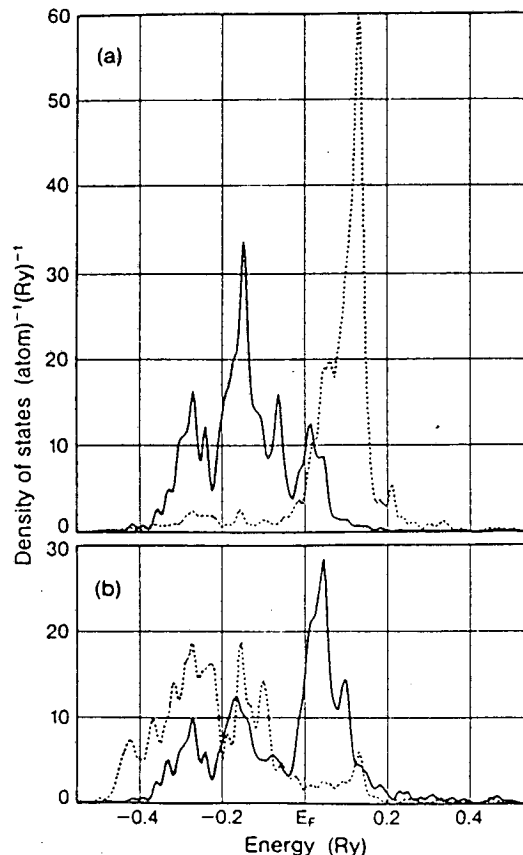
Magnetic surface effects [17] are particularly challenging. They arise from collective behavior, and require special care in treating selfconsistently the electron-electron interaction.

Figure 2. Comparison between peak positions in angle-resolved photoemission experiments [13,14] performed on cleaved Si (111) - (2 × 1) and a theoretical calculation [15] based on a π -bonded model of the rearranged dangling bonds. Data are plotted versus \vec{k}_{\parallel} . The experimental points are the squares [13] and circles [14]; the continuous line is the theoretical results [15]. The shaded area corresponds to occupied bulk states.



Among the most interesting cases recently studied is antiferromagnetic chromium [17-20]. In its bulk form chromium is a body-centered cubic transition-metal which exhibits an oscillating magnetization (a spin-density wave) with a period of about 25 lattice spacings and a maximum value of 0.59 Bohr magnetons. When a $\langle 100 \rangle$ surface is created, the structure remains antiferromagnetic, with all the atoms on the surface layer having a parallel magnetization (ferromagnetic surface). This magnetization is in turn antiparallel to that of the second-layer atoms. The surprising result, however, is that the presence of the surface produces a very large *enhancement* of the surface layer magnetization, which attains values between 2.4 and 3.0 Bohr magnetons. This enhancement decays exponentially from the surface into the bulk, with a factor of approximately 2 -- and a sign alternation -- between consecutive layers. The calculated [18] values of the magnetization in the first five layers are 3.00, -1.56, 1.00, -0.93, and 0.86. From these numbers it is obvious that photoemission experiments in chromium can never provide information on the "true" bulk material, since the magnetic rearrangement at the surface is so deep as to influence all the photoemitted electrons, regardless of the radiation frequency employed. All these traits of the Cr (100) surface have been confirmed experimentally.

Figure 3. The projected density of d -states for a (100) monolayer of chromium on iron. (a) The chromium (100) monolayer. (b) The iron (100) interface layer. Solid lines are states with the spin orientation of the minority bulk iron states; dashed lines correspond to the majority states. The overlayer has a huge magnetization of 3.63 Bohr magnetons (an enhancement of over a factor of 6 from the chromium bulk value), and is *antiferromagnetically* oriented with respect to the iron. The iron interface layer has its magnetization reduced from the iron bulk value of 2.2 to 1.95 Bohr magnetons.



The magnetic rearrangement situation can be even more complicated when two-component magnetic samples are prepared. Figure 3 shows the projected density of states, separated by spin orientation, for the case of a monolayer of chromium on the (100) surface of iron: in this particular case the chromium arranges itself in a *ferromagnetic* overlayer, oriented *antiferromagnetically* with respect to the iron substrate.

DYNAMIC MANY-BODY EFFECTS

Not all photoemission spectra can, however, be explained on the basis of one-electron calculations, even if the latter are self-consistent and take into account many-body effects in the best possible "average" way. Photoemission is a dynamic process and the nature of the phenomenon requires that, in many instances, collective many-body effects -- inaccessible by mean-field approaches -- do play an active role. Under those conditions, understanding the experimental data requires a more complicated theoretical treatment. It should be remember at all times, however, that even if dynamic many-body effects must be introduced to explain a given result, in practically all instances the effect is either dominated, or drastically influenced, by the one-particle structure discussed in the previous sections.

Good examples of this interplay of one-body and many-body effects can be found in strongly correlated solids: the transition metals, the rare earths, magnetic compounds, fluctuating-valence solids, heavy fermions, density-wave materials, etc. A good and frequently mentioned case is metallic nickel. It is a simple 3-*d* transition metal, an itinerant ferromagnet whose electronic band structure is well known [5, 21], has been measured by several Fermi surface techniques, as well as by angle-resolved photoemission [10, 22-24] and checked against theoretical results [21], and which is known to have small but detectable magnetic rearrangement effects at surfaces and interfaces [16]. The detailed agreement between theory and experiment is excellent. There are however four features of the photoemission data that cannot be explained by simple one-electron calculations:

- (1) Core-level photoemission exhibits satellites approximately 6 eV below the main lines [25-27];
- (2) Resonant photoemission is observed for photon energies of approximately 67 eV [28-30];
- (3) There is a resonant satellite in the valence band, approximately 6 eV below the Fermi level [24, 28];
- (4) Valence band photoemission shows an apparent *d*-band width and exchange splittings reduced by 25% and 50%, respectively [22-24], relative to the calculated one-electron band structure [21, 31] (see Figure 4).

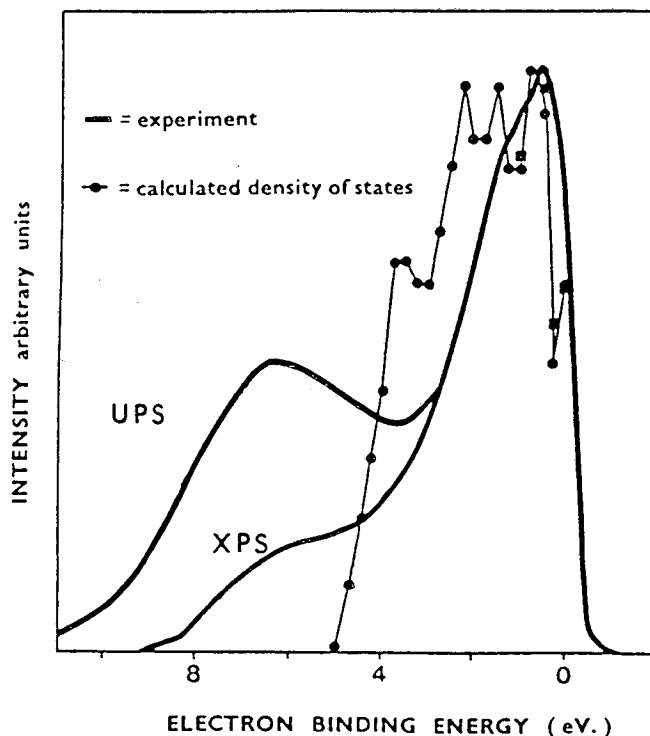


Figure 4.- Comparison between the calculated density of one-electron states for nickel [21] and the valence-band photoemission spectra in the ultra-violet (UPS) and the X-ray (XPS) regimes [31].

Several excellent treatments of the many-body problem have been published [31-39]. However, in order to take good account of the complicated many-body perturbation calculation, most of them resort to simplified band structures (e.g. free-electron-like bands) which tend to make comparison with experiment either difficult or even impossible. A more realistic approach has been proposed by Victora and Falicov [39], who have resorted to a small-periodic-cluster approach. This approach reduces the sampling of the Brillouin Zone to only a few points (four in their calculation), but -- within the restricted sampling set -- the problem is treated *exactly*, and both *one-electron* and *many-body* aspects are considered *on an equal footing*.

Victora and Falicov [39] considered a four-atom tetrahedral cluster with periodic boundary conditions -- a micro face-centered cubic crystal. They included ten electron orbitals per site, used the one-electron energy parameters of Wang and Callaway [21], and considered full intra-atomic electron-electron interactions between the various *d*-orbital electrons. Atomic symmetry allows for three independent intra-atomic interaction parameters, normally labelled *U*, *J*, and ΔJ , which they kept in the ratio 56:8:1, and which they scaled to obtain the proper satellite spectral position. A value of *U* = 4.3 eV yielded the best results.

The cluster of 4 sites contains 40 *d*-orbitals; 38 electrons (2 holes) were included in the ground state, yielding an average occupancy of 9.5 *d*-electrons per atom, very close to the observed [40] value of 9.46. For two holes the tetrahedral cluster with the characteristics described above has an analytically expressed ground state. This state -- of symmetry 3X_2 -- contains only holes in the X_5 , minority-spin one-electron orbitals. Because of the Pauli exclusion principle it has zero probability of having two holes in one site: the holes are (through exchange) perfectly correlated with one another, and consequently, counting from the full *d*-shell, there is no contribution to the ground-state energy from the one-site, hole-hole interaction.

The photoemission process introduces a third hole into the system. The three-hole manifold of the tetrahedral cluster contains 9880 many-body states. The use of group theory simplifies the matrix considerably: the largest secular problem to solve, once group factorization had been accomplished, is of order 238. If final-state effects (such as variations in the density of the emitted-electron states, or resonance effects involving core electrons) are neglected, the observed, non-resonant density of photoemission states -- the X-ray photoemission spectrum XPS -- is obtained by projecting the analytic 3X_2 -ground-state with an extra hole into the three-hole energy-eigenvalue spectrum. By selecting the desired one-electron-orbital *k*-vector, space and spin symmetries of the extra hole (the photoemitted electron), angular resolution (only *k*-vectors at Γ and *X* can be calculated because of the restricted sampling), spin polarization and spatial distribution spectra can be determined.

Figure 5.
The total density of calculated emitted one-electron states in metallic nickel [39]. The location of the lowest single-electron state at *X* in the *d*-band according to band-structure calculations [21] is denoted by E_0 .

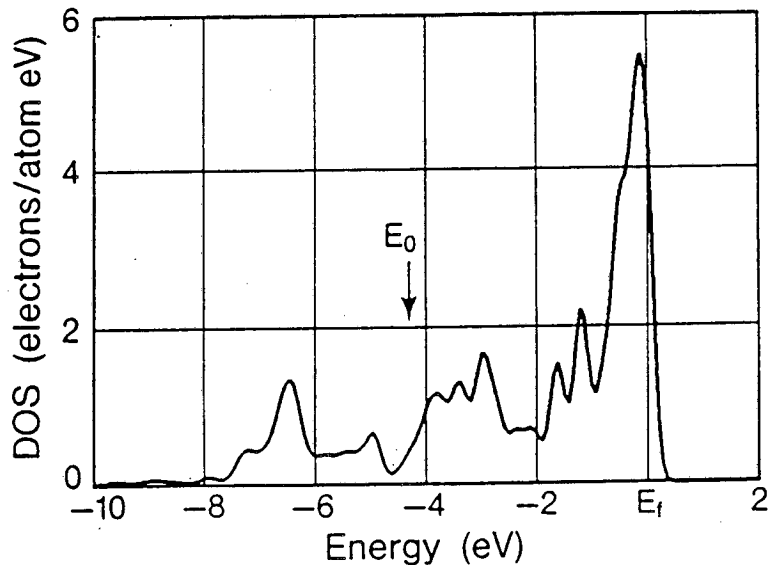


Figure 6.
Density of emitted states
in metallic nickel,
projected on the wave
vector and symmetry of the
emitted electron [39].
Solid lines correspond to
minority-spin states;
dashed lines are for
majority-spin states.

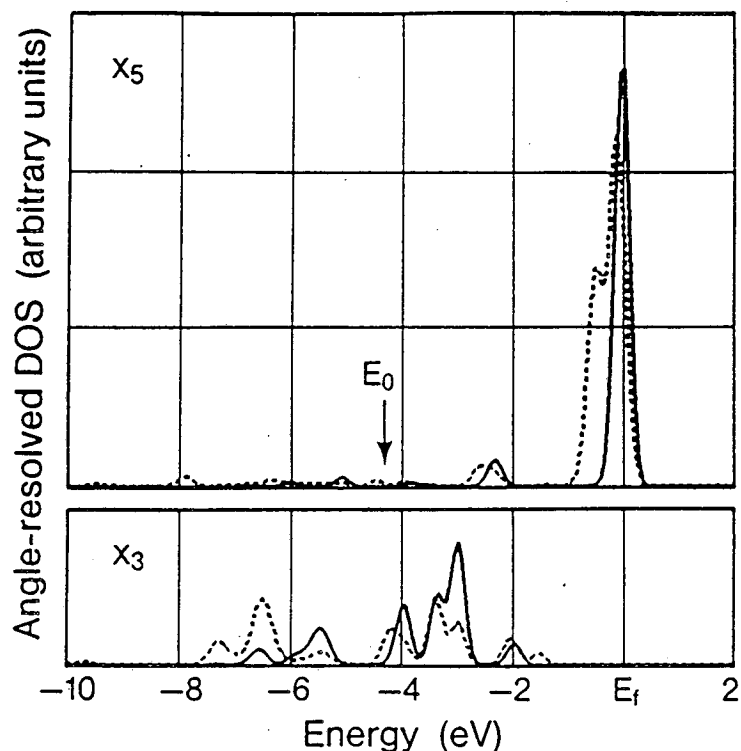


Figure 5 shows angle-, symmetry- and spin-integrated results. The discrete spectrum of 9880 lines has been broadened with a narrow Gaussian of 0.15 eV half-width. It compares well with experiment not only in the existence of a satellite, but in its relative intensity with respect to the main band of the spectrum. Projected densities of emitted states with symmetries X_5 and X_3 for the photoelectron are shown in Figure 6. States of X_5 symmetry, near the Fermi level, are characterized by single, narrow peaks. States of X_3 symmetry, near the bottom of the band, have strong satellite components and exhibit a well known multiplet structure.

The results yield the following conclusions:

- (i) three-hole eigenstates corresponding to the "main band" have a greatly reduced probability of finding two holes in the same atom (20% at the Fermi level, 5% at the bottom of the band), as opposed to 50% in a random state created from the 3X_2 ground state;
- (ii) three-hole eigenstates in the satellite part of the spectrum have a very high probability of finding two holes in one atom;
- (iii) the many-body calculation yields a considerably reduced bandwidth of 3.4 eV, in excellent agreement with the experimental [22-24] value of 3.3 eV, and considerably reduced from the band-structure [21] value of 4.3 eV;
- (iv) band-structure calculations yield a Fermi-level X_5 line which consists only of majority-spin electrons -- the corresponding minority-spin states are above the Fermi level, i.e. empty; the results of Figure 4 clearly point out that the X_5 Fermi-level line is a combination of both spins, that the minority X_5 states are appreciably occupied in the true many-body states, and that the exchange splitting of that X_5 level is very small [41];
- (v) agreement with experimentally determined values of the spectral lines is very good throughout, with the exception -- similar to previous work [34] -- of the energy of the assigned X_2 symmetry.

Similar calculations have been performed for ferromagnetic iron [42], and can be extended, albeit laboriously, to other transition-metal and rare-earth compounds [43].

PROJECTION

The future looks very bright for the continuation of this type of research, an intrinsically interwoven fabric of careful experiments and realistic, detailed calculations. Comparison between angle-resolved photoemission data and one-electron calculations -- both bulk and surface -- will continue to be a matter that, even

though routine, will still require careful experimentation, insightful interpretation of the data, accurate calculations and sophisticated matching of theory and experiment.

As the experiments progress and new effects are found, determined and/or measured, there will be more need for calculations that go beyond the one-particle approach. Inclusion of many-body, dynamic effects on the same footing as the one-electron terms will be necessary, and the required calculations [44] will heavily tax the imagination and ingenuity of the theoretical physicist, as well as the computational resources -- memory, accessibility and speed -- that, fortunately, are becoming every day more plentiful and affordable.

ACKNOWLEDGMENTS

The author wishes to thank his collaborators, L. Klebanoff, D. A. Shirley, A. Reich, E. C. Sowa, and R. H. Victora for their many valuable contributions. This research was supported, in part, at the Lawrence Berkeley Laboratory, by the Director, Office of Energy Research, Materials Science Division, U.S. Department of Energy, under contract No. DE-AC03-SF00098. The superb hospitality of NORDITA and the H. C. Ørsted Institute during the author's stay in Copenhagen is acknowledged with thanks.

REFERENCES

- [1] CARDONA, M. and LEY, L., *Photoemission in Solids* (Springer Verlag, Berlin, Heidelberg, New York), *Volume I: General Principles* (1978), *Volume II: Case Studies* (1979).
- [2] COHEN, M. L., *Nature* **234** (1986) 549-553.
- [3] EINSTEIN, A., *Ann. Physik* **17** (1905) 132-148.
- [4] SMITH, N. V., reference [1], Volume I, pp. 237-264.
- [5] MORUZZI, V. L., JANAK, J. F., and WILLIAMS, A. R., *Calculated Electronic Properties of Metals*, (Pergamon, New York, 1978).
- [6] ANDERSEN, O. K., JEPSEN, O., and GLÖTZEL, in *Highlights of Condensed-Matter Theory*, edited by F. Bassani, F. Fumi, and M. P. Tosi (North-Holland, New York, 1985) pp. 59-176.
- [7] COHEN, M. L., *Physica Scripta T1* (1982) 5-10.
- [8] BURDICK, G. A., *Phys. Rev.* **129** (1963) 138-150.
- [9] THIRY, P., CHANDESRIS, D., LECANTE, J., GUILLOT, C., PINCHAUX, R. and PETROFF, Y., *Phys. Rev. Lett.* **43** (1979) 82-85.
- [10] HIMPSEL, F. J., *Adv. Phys.* **32** (1983) 1-51.
- [11] SHIRLEY, D. A., reference [1], Volume I, pp. 165-195.
- [12] LOUIE, S. G., THIRY, P., PINCHAUX, R., PETROFF, Y., CHANDESRIS, D., and LECANTE, J., *Phys. Rev. Lett.* **44** (1980) 549-553.
- [13] HIMPSEL, F. J., HEIMANN, P., and EASTMAN, D. E., *Phys. Rev. B* **24** (1981) 2003-2008.
- [14] UHRBERG, R. I., HANSSON, G. V., NICHOLLS, J. M., and FLOSTRÖM, S. A., *Phys. Rev. Lett.* **48** (1982) 1032-1035.
- [15] PANDEY, K. C., *Physica B* **117-118** (1983) 761-766.
- [16] TERSOFF, J., and FALICOV, L. M., *Phys. Rev. B* **26** (1982) 6186-6200.
- [17] FALICOV, L. M., and MORAN-LOPEZ, J. L., *Magnetic Properties of Low-Dimensional Systems* (Springer Verlag, Berlin, Heidelberg, New York, 1986).
- [18] VICTORA, R. H., and FALICOV, L. M., *Phys. Rev. B* **31** (1985) 7335-7343.
- [19] KLEBANOFF, L. E., VICTORA, R. H., FALICOV, L. M., and SHIRLEY, D. A., *Phys. Rev. B* **32** (1985) 1997-2005.
- [20] KLEBANOFF, L. E., ROBEY, S. W., LIU, G., and SHIRLEY, D. A., *Phys. Rev. B* **30** (1984) 1048-1051.
- [21] WANG, C. S., and CALLAWAY, J., *Phys. Rev. B* **15** (1977) 298-306.
- [22] EASTMAN, D. E., HIMPSEL, F. J., and KNAPP, J. A., *Phys. Rev. Lett.* **40**, (1978) 1514-1517.
- [23] HIMPSEL, F. J., KNAPP, J. A., and EASTMAN, D. E., *Phys. Rev. B* **19**, (1979) 2919-2927.
- [24] EBERHARDT, W., and PLUMMER, E. W., *Phys. Rev. B* **21**, (1980) 3245-3255.
- [25] BAER, Y., HEDEN, P. F., HEDMAN, J., KLASSON, M., NORDLING, C., and SIEGBAHN, K., *Physica Scripta* **1**, (1970) 55-65.
- [26] HUFNER, S., and WERTHEIM, G. K., *Phys. Lett.* **51A**, (1975) 299-300.
- [27] FELDKAMP, L. A., and DAVIS, L. C., *Phys. Rev. B* **22**, (1980) 3644-3653.
- [28] GUILLOT, C., BALLU, Y., PAIGNE, J., LECANTE, J., JAIN, K. P., THIRY, C., PINCHAUX, R., PETROFF, Y., and FALICOV, L. M., *Phys. Rev. Lett.* **39** (1977) 1632-1635.
- [29] CLAUSBERG, R., GUDAT, W., KISKER, E., KUHLMANN, E., and ROTHBERG, G. N., *Phys. Rev. Lett.* **47**, (1981) 1314-1317.

- [30] FELDKAMP, L. A., and DAVIS, L. C., Phys. Rev. Lett. 43, (1979) 151-154.
- [31] PENN, D. R., Phys. Rev. Lett. 42 (1979) 921-925.
- [32] TREGLIA, G., DUCASTELLE F., and SPANJAARD D. Phys. Rev. B 21, (1980) 3729-3733.
- [33] LIEBSCH, A., Phys. Rev. Lett. 43 (1979) 1431-1434.
- [34] LIEBSCH, A., Phys. Rev. B 23 (1981) 5203-5212.
- [34] DAVIS, L. C., and FELDKAMP, L. A., Solid State Commun. 34, (1980) 141-145.
- [35] MARTENSSON, N., and JOHANSSON, B., Phys. Rev. Lett. 45, (1980) 482-485.
- [36] KLEINMAN, L., and MEDNICK, K., Phys. Rev. B. 24, (1981) 6880-6888.
- [37] CLAUSBERG, R., Phys. Rev. B 28, (1983) 2561-2565.
- [38] AISAKA, T., KATO, T., and HAGA, E., Phys. Rev. B 28, (1983) 1113-1116.
- [39] VICTORA, R. H., and FALICOV, L. M., Phys. Rev. Lett. 55 (1985) 1140-1143.
- [40] DANAN, H., HEER, R., and MEYER, A. P. J., J. Appl. Phys. 39 (1968) 669-670.
- [41] GUDAT, W., KISKER, E., KUHLMANN, E., and CAMPAGNA, M., Phys. Rev. B 22 (1980) 3282-3287.
- [42] SOWA, E. C., and FALICOV, L. M., Phys. Rev. B 35 (1987) 3765-3772.
- [43] REICH, A., and FALICOV, L. M., Phys. Rev. B 34 (1986) 6752-6758.
- [44] BARDYSZEWSKI, W., and HEDIN, L., Physica Scripta 32 (1985) 439-450.

LAWRENCE BERKELEY LABORATORY
TECHNICAL INFORMATION DEPARTMENT
UNIVERSITY OF CALIFORNIA
BERKELEY, CALIFORNIA 94720